Introduction to Diffusion Models (October 10, 2023)

Santiago VELASCO-FORERO
http://cmm.ensmp.fr/~velasco/

MINES Paris
PSL Research University
Center for Mathematical Morphology

Contents

1. Introduction
2. Generative models
   - Classical Generative Modeling
   - Autoencoders
   - Variational Autoencoder
3. Generative Adversarial Networks (GANs)
4. Variational Diffusion Models
5. References

Contents

1 Introduction

2 Generative models

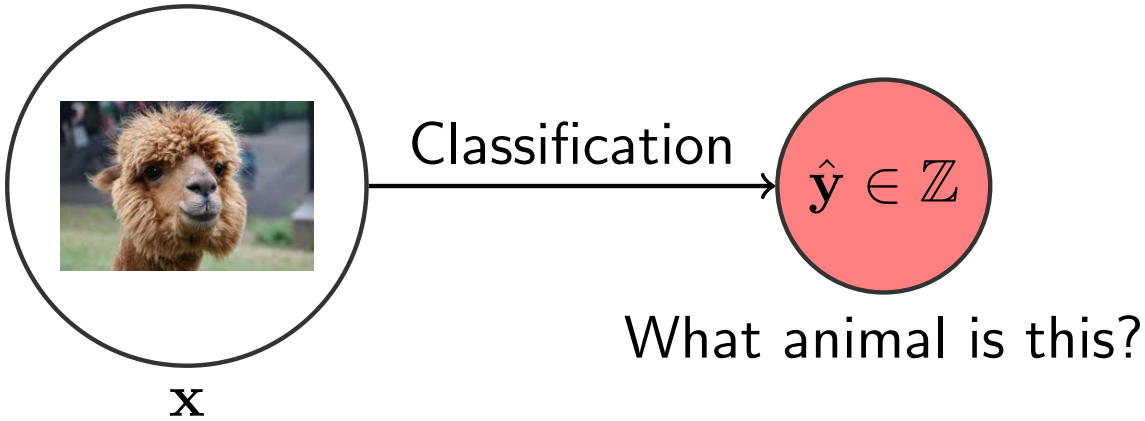
3 Generative Adversarial Networks (GANs)

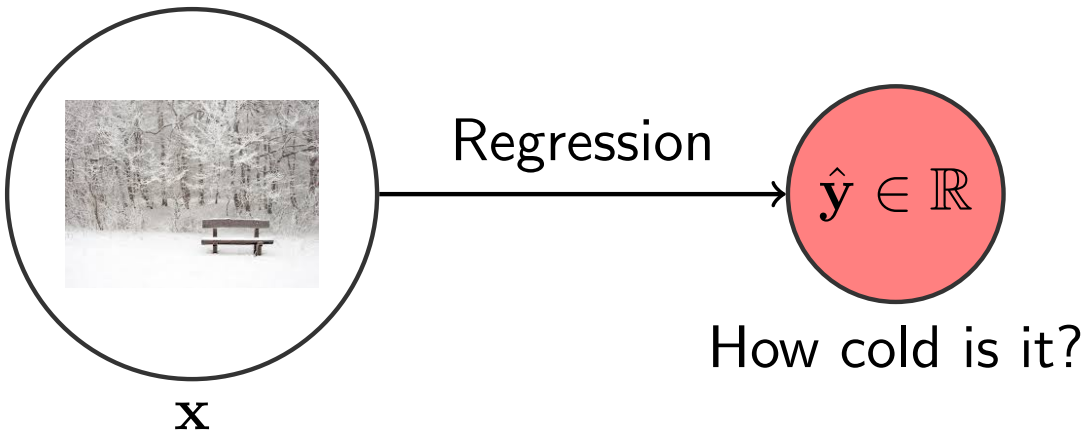
4 Variational Diffusion Models

5 References

Supervised Learning

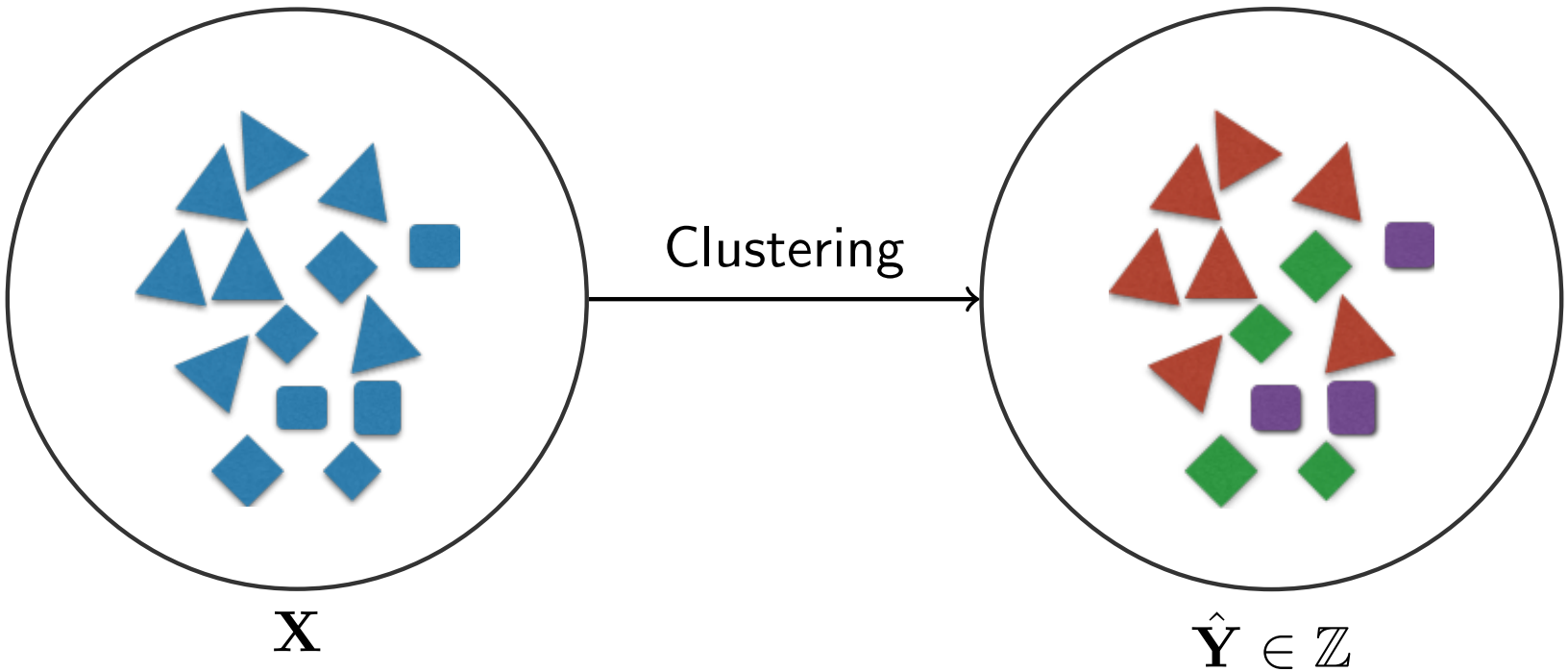
Given a labeled dataset $(\mathbf{X}, \mathbf{Y})$, we would like to learn a mapping from data space to label space.





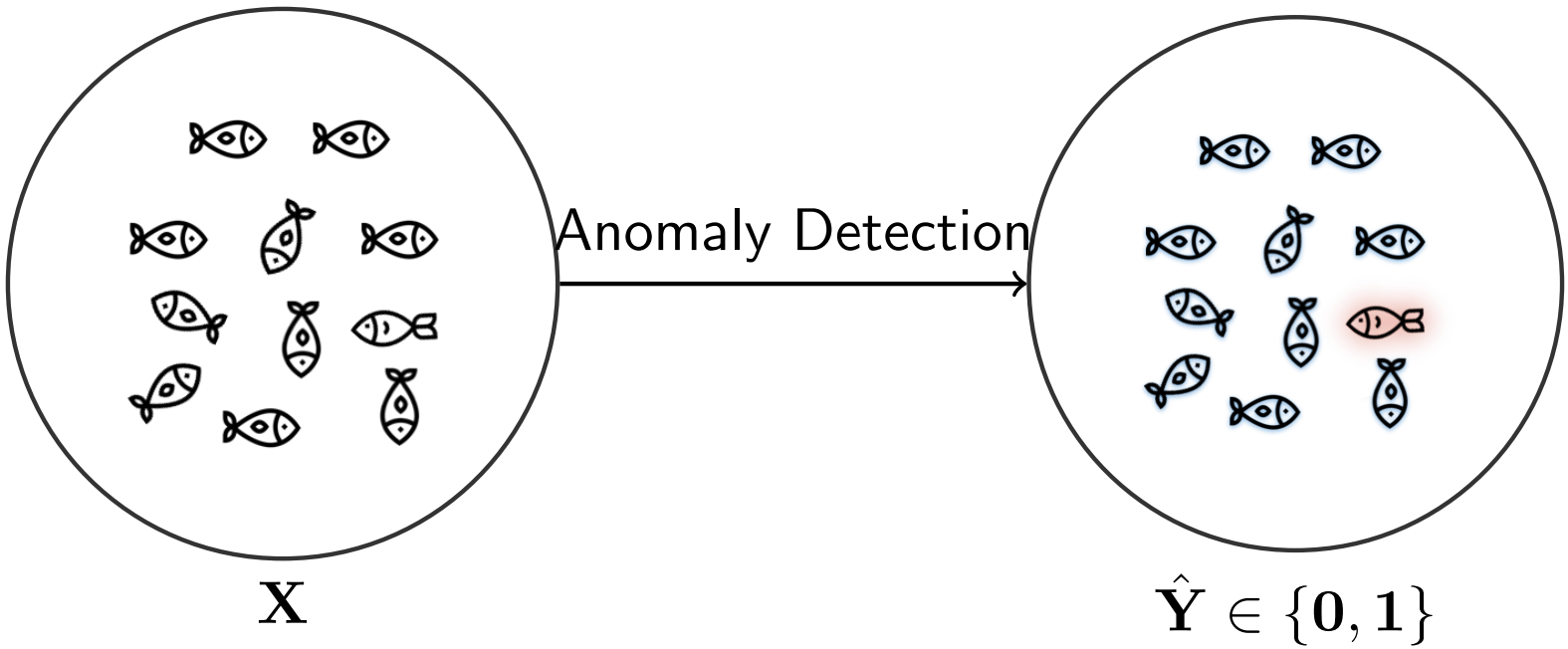
Unsupervised Learning: Clustering

Given an unlabeled dataset $(\mathbf{X})$, we would like to learn: How to group objects into categories?



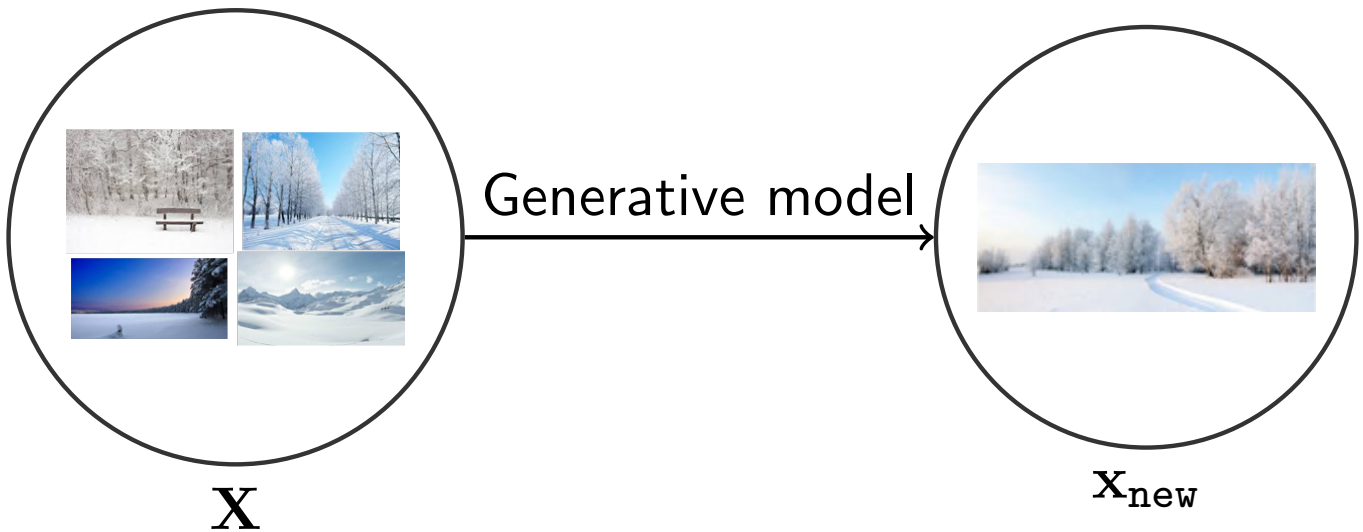
Anomaly detection

Given an unlabeled dataset $(\mathbf{X})$, we would like to learn: How to identify observations differing significantly from the majority of data?



Unsupervised learning: Generative Models

Given an unlabeled dataset $(\mathbf{X})$, we would like to learn: How to generate a new observation from the same distribution (unknown) of dataset?



Contents

1. Introduction
2. Generative models
   - Classical Generative Modeling
   - Autoencoders
   - Variational Autoencoder
3. Generative Adversarial Networks (GANs)
4. Variational Diffusion Models
5. References

Goal

Generative models "learn" a joint distribution over a dataset. They are mostly used for sampling applications or density estimation.

1. (Sampling) A generative model learns to fit a model over observations so one can sample novel data from the model, $\mathbf{x}_{new} \sim p_{\boldsymbol{\theta}}(\mathbf{x})$
2. (Density estimation) A model learns to estimate the probability of observations. Given a datapoint $\mathbf{x}$ the model, what is the probability of $\mathbf{x}$ belong to the dataset?

Generative models

- Given observed samples i.i.d. $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ from a distribution of interest (unknown) in $\mathbb{R}^p$, the goal of a *generative model* is to learn to model its true data distribution $p(\mathbf{x})$.

Generative models

- Given observed samples i.i.d. $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ from a distribution of interest (unknown) in $\mathbb{R}^p$, the goal of a *generative model* is to learn to model its true data distribution $p(\mathbf{x})$.
- After learning, we can *generate* new samples from our approximate model.
- In most of the applications, one is interested in conditional generative models, for instance, generate an image from a text, or generate an image from another image, so on.

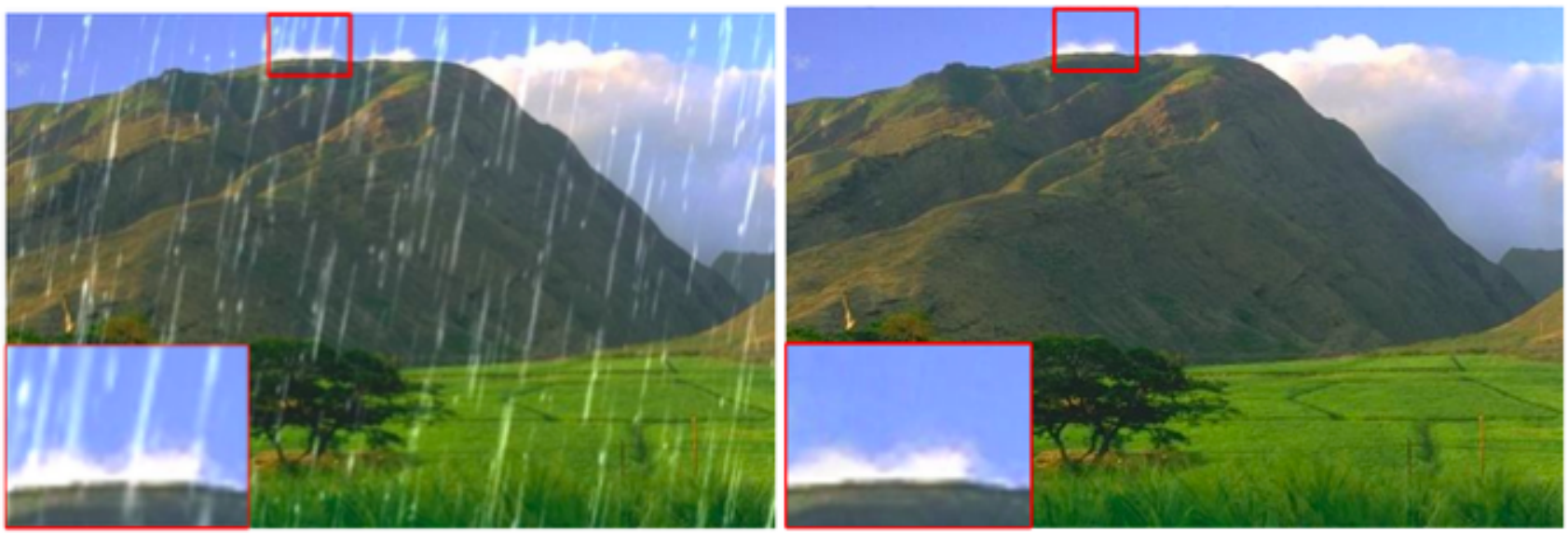
Examples of Conditional generation.

1. Face Frontal View Generation

2. Photos to Emojis
3. Image Editing
4. Image De-raining
5. Text-to-Image
6. Many others...

Examples of Conditional generation.

1. Face Frontal View Generation
2. Photos to Emojis
3. Image Editing
4. Image De-raining

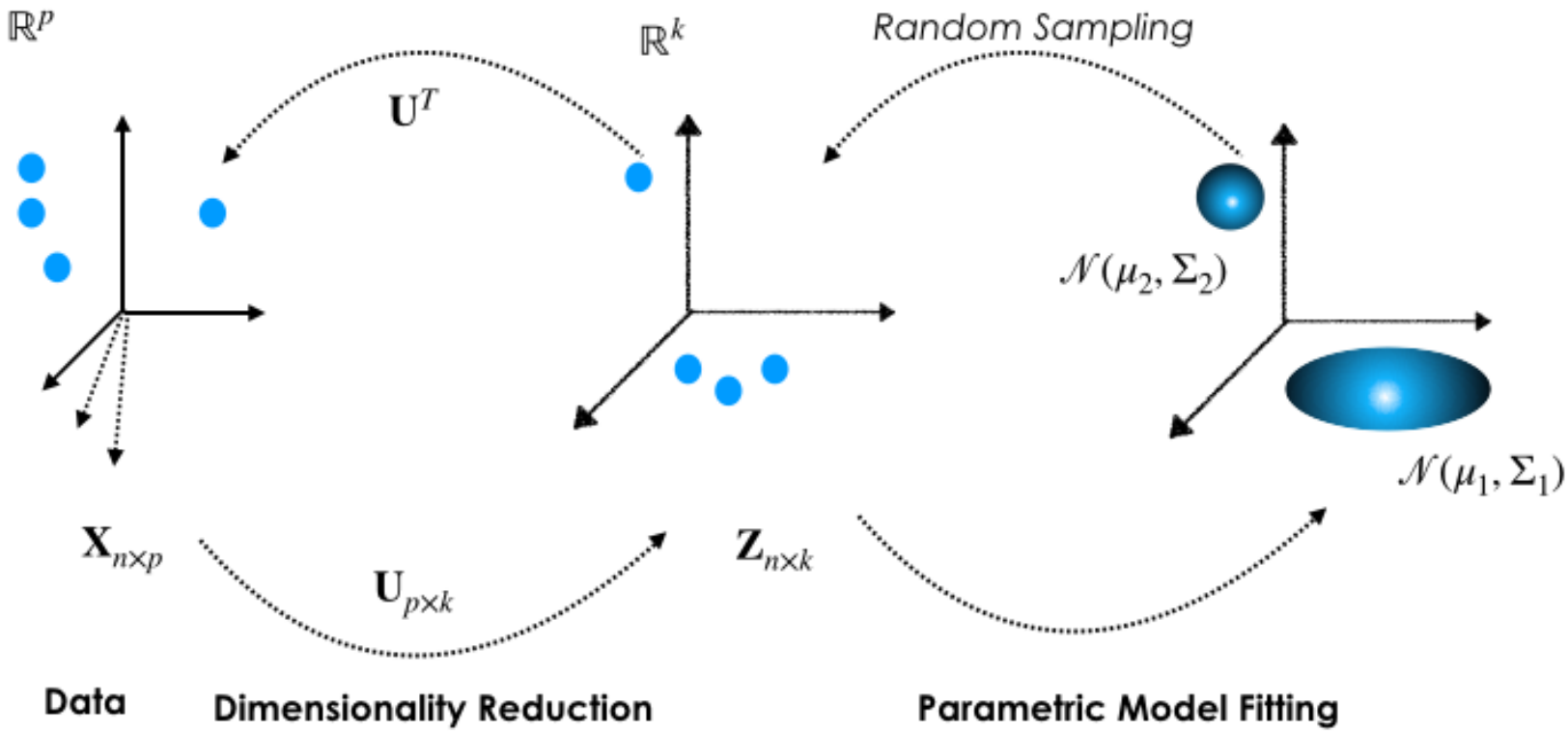


5. Text-to-Image
6. Many others...

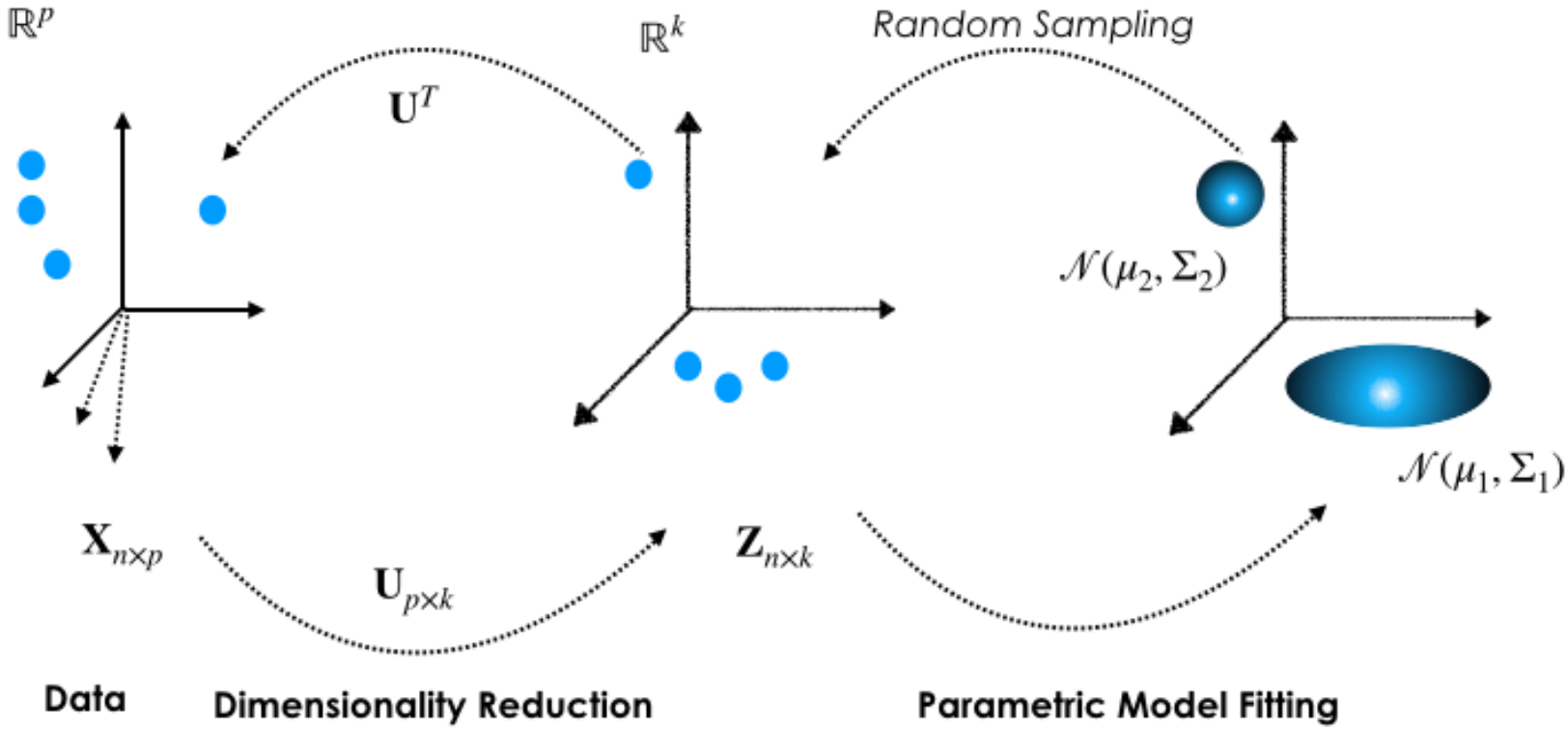
Contents

1. Introduction
2. Generative models
   - Classical Generative Modeling
   - Autoencoders
   - Variational Autoencoder
3. Generative Adversarial Networks (GANs)
4. Variational Diffusion Models
5. References

Classical Generative Modeling

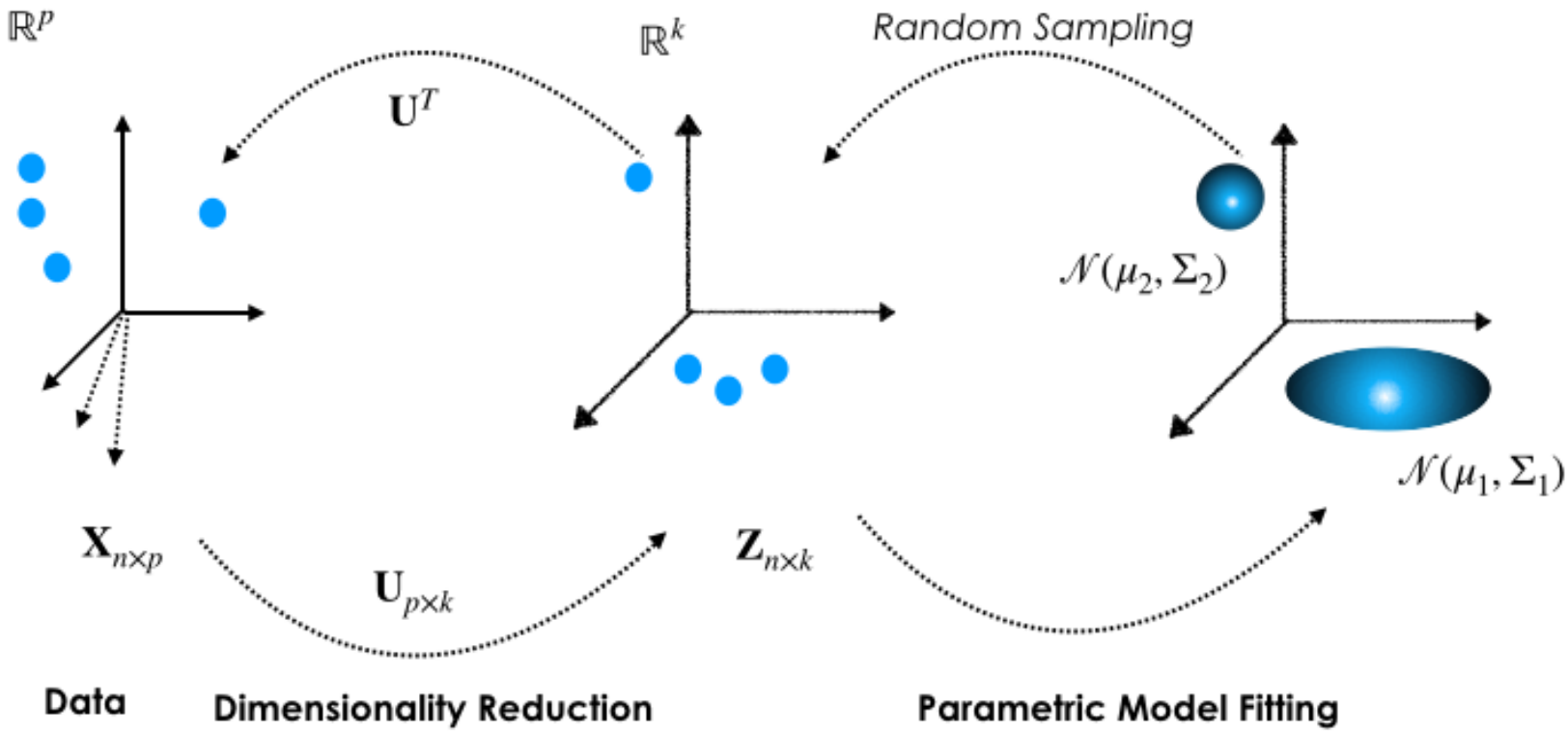


Classical Generative Modeling



- Dimensionality reduction: Usually linear by maximal variance subspace (Principal Component Analysis)
- Distribution Modeling: Usually Mixed Multivariate Gaussian Distribution

Classical Generative Modeling



Limitations:

- Nonlinear relations are difficult to be considered. For instance: Spatial Correlation between Pixels.
- Distribution Modeling: Fitting parametric models in high-dimensions is hard. *Curse of Dimensionality*

Generative models

- Given observed samples i.i.d. $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ from a distribution of interest (unknow) in $\mathbb{R}^p$, the goal of a *generative model* is to learn to model its true data distribution $p(\mathbf{x})$.
- After learning, we can *generate* new samples from our approximate model.
- Closed form for the model is not required

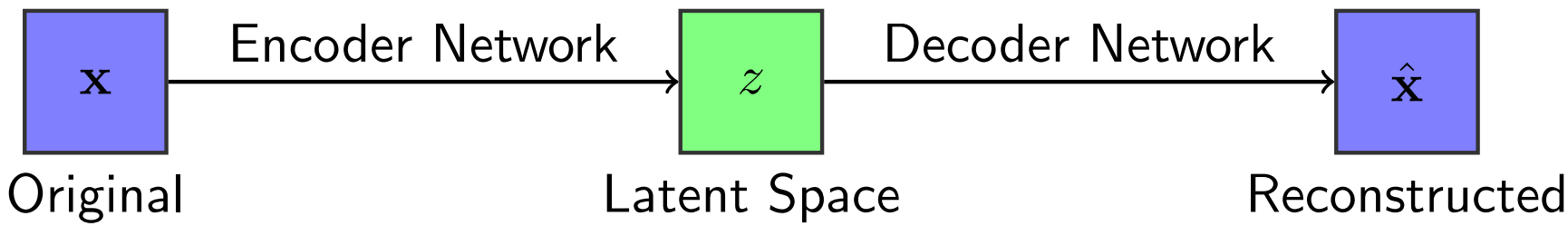
Contents

1. Introduction
2. Generative models
   - Classical Generative Modeling
   - Autoencoders
   - Variational Autoencoder
3. Generative Adversarial Networks (GANs)
4. Variational Diffusion Models
5. References

Autoencoders

Autoencoders are neural networks whose purpose is twofold:

1. To compress some input data by transforming it from the input domain to another space, known as the *latent space* (code).
2. To take this latent representation and transform it back to the original space, such that the output is *similar* to the input.



The loss function for a given input vector is usually the reconstruction error:

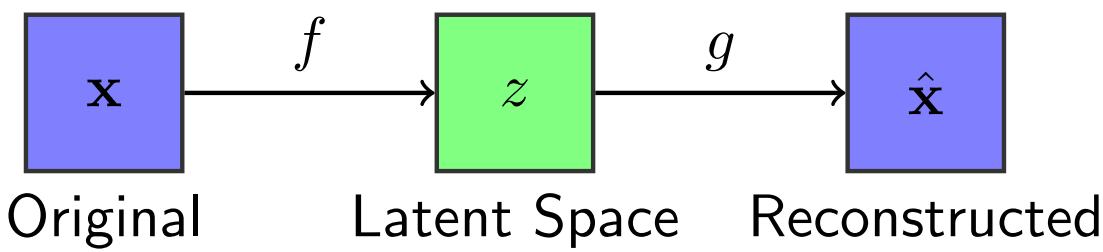
$$L(\mathbf{x}) = \|\mathbf{x} - \hat{\mathbf{x}}\|^2$$

Autoencoder

- An *autoencoder* is a neural network that is trained to attempt to copy its input to its output.
- The network may be viewed as consisting of two parts: an encoder function $z = f(\mathbf{x})$ and a decoder that produces a reconstruction $r(\mathbf{x}) = g(f(\mathbf{x}))$.
- The composition of f and g is called the *reconstruction function*
- If an autoencoder succeeds to learn $g(f(\mathbf{x})) = \mathbf{x}$ everywhere, then it is not especially useful (overfitting).
- The learning process consists in minimizing the loss function:

$$L(\mathbf{x}, g(f(\mathbf{x}))), \tag{1}$$

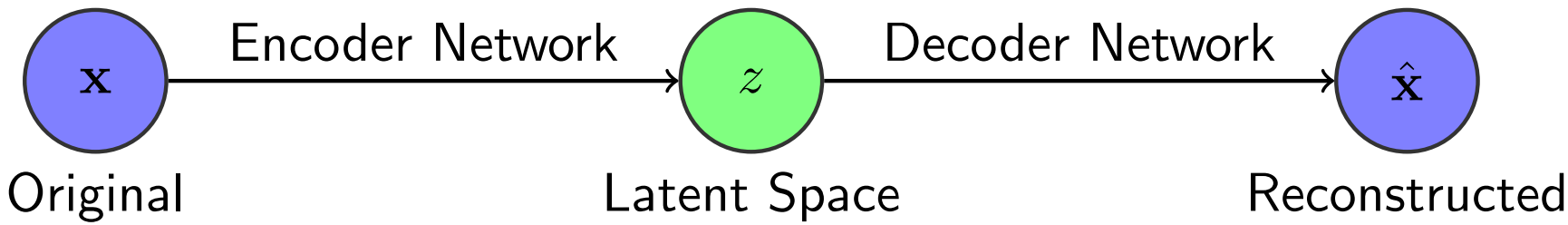
where L is a loss function, such as mean squared error.



Autoencoders

Autoencoders are neural networks whose purpose is twofold:

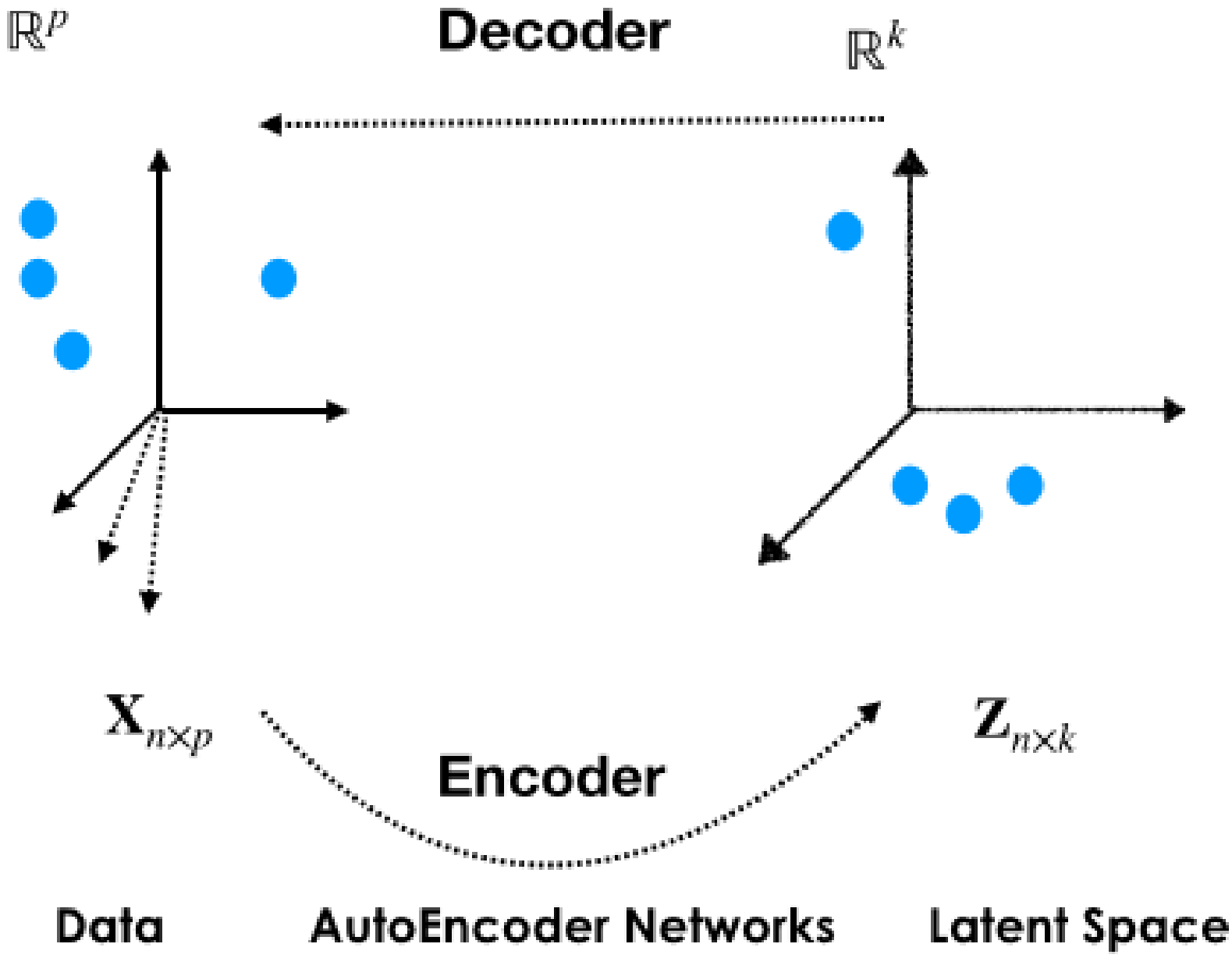
1. To compress some input data by transforming it from the input domain to another space, known as the *latent space* (code).
2. To take this latent representation and transform it back to the original space, such that the output is *similar* to the input.



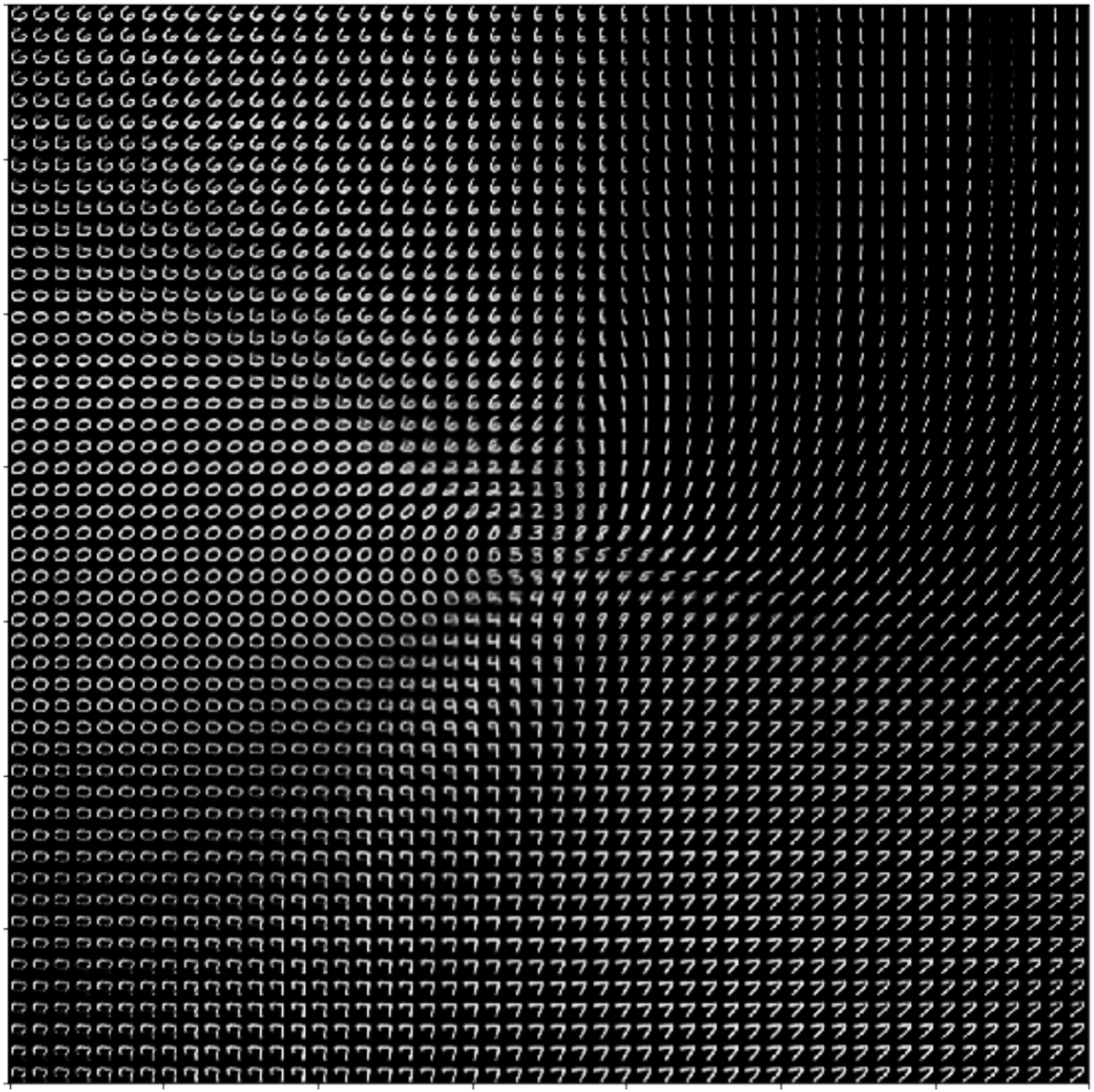
The loss function for a given input vector is usually the reconstruction error:

$$L(\mathbf{x}) = \|\mathbf{x} - \hat{\mathbf{x}}\|^2$$

AutoEncoder Scheme



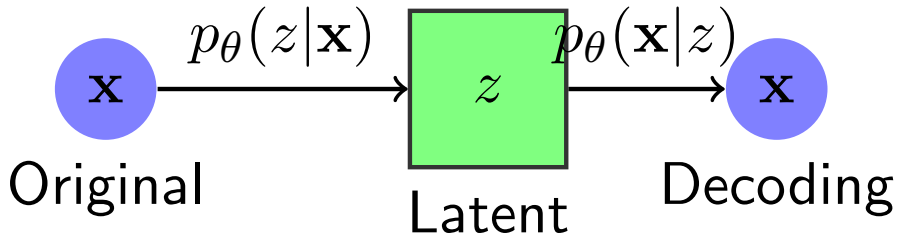
Example: $k = 2$, latent space for MNIST dataset



Contents

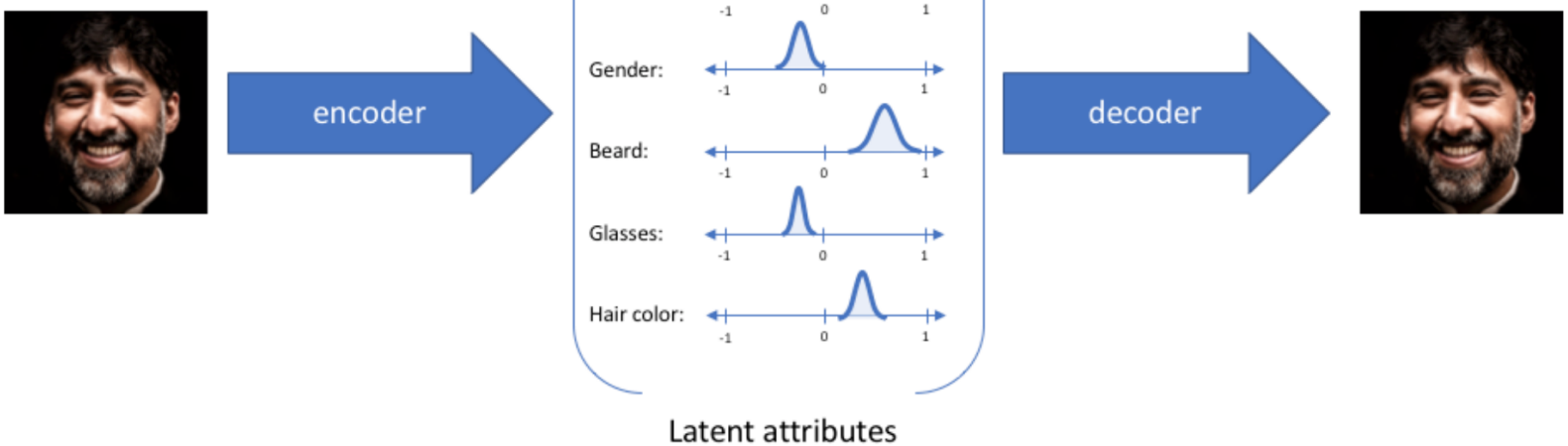
1. Introduction
2. Generative models
   - Classical Generative Modeling
   - Autoencoders
   - Variational Autoencoder
3. Generative Adversarial Networks (GANs)
4. Variational Diffusion Models
5. References

Variational Autoencoder



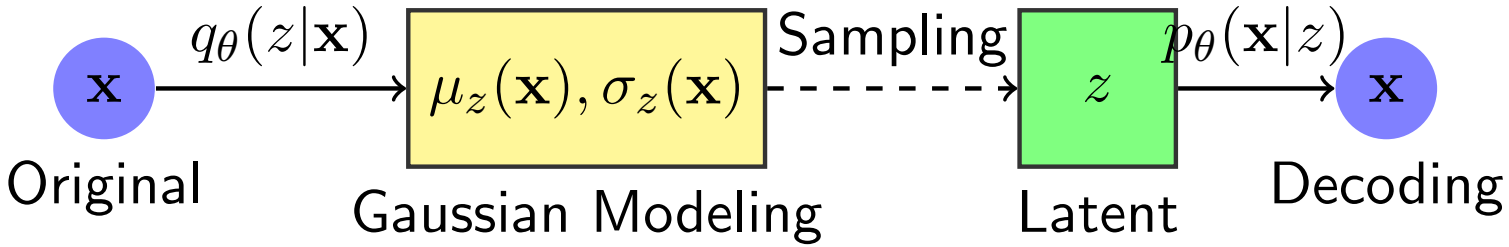
- Training via maximum likelihood of $p(\mathbf{x})$
- Intractability: the true posterior density $p_\theta(z|\mathbf{x})$ cannot be calculated in polynomial time
- Solution: Approximate $p_\theta(z|\mathbf{x})$ by means of $q_\theta(z|\mathbf{x}) = \mathcal{N}(z; \mu_z(x), \sigma_z(x))$

Latent space intuition (variational case)



Credits:
https://www.jeremyjordan.me/variational-autoencoders/

Variational Autoencoder



- Gaussian modeling
- Training via maximum likelihood of $p(\mathbf{x})$
- Learning the parameters θ via backpropagation?

Training via maximum likelihood

Assume we would like to compute the likelihood of an image $\mathbf{x}$ from the training set:

$$
\begin{aligned}
\mathcal{L}(\mathbf{x}) &= \log(p(\mathbf{x})) \\
&= \sum_z q(z|\mathbf{x}) \log(p(\mathbf{x})) \\
&= \sum_z q(z|\mathbf{x}) \log\left(\frac{p(z,\mathbf{x})}{p(z|\mathbf{x})}\right) \\
&= \sum_z q(z|\mathbf{x}) \log\left(\frac{p(z,\mathbf{x})q(z|\mathbf{x})}{q(z|\mathbf{x})p(z|\mathbf{x})}\right) \\
&= \sum_z q(z|\mathbf{x}) \log\left(\frac{p(z,\mathbf{x})}{q(z|\mathbf{x})}\right) + \sum_z q(z|\mathbf{x}) \log\left(\frac{q(z|\mathbf{x})}{p(z|\mathbf{x})}\right) \\
&= \sum_z q(z|\mathbf{x}) \log\left(\frac{p(z,\mathbf{x})}{q(z|\mathbf{x})}\right) + \underbrace{D_{KL}(q(z|\mathbf{x}), p(z|\mathbf{x}))}_{\geq 0}
\end{aligned}
$$

Kullback-Leibler Divergence

They introduced the concept of the KL divergence in 1951.

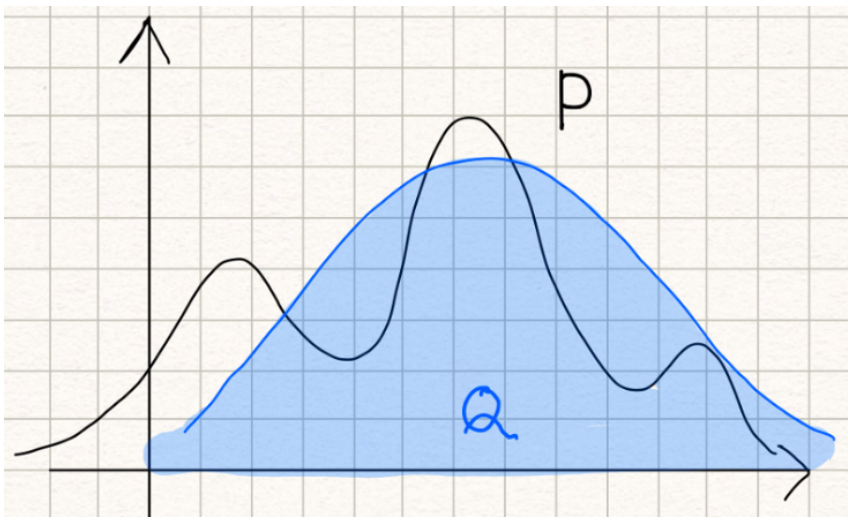
$$D_{KL}(p||q) = \int p(x) \log \frac{p(x)}{q(x)} dx \tag{2}$$

Kullback-Leibler Divergence

They introduced the concept of the KL divergence in 1951.

$$D_{KL}(p||q) = \int p(x) \log \frac{p(x)}{q(x)} dx \tag{2}$$

- KL divergence is non-negative
- KL divergence is asymmetric
- $D_{KL}(p||q) = \mathbb{E}_{x \sim p(x)} \log \frac{p(x)}{q(x)}$



Training via maximum likelihood

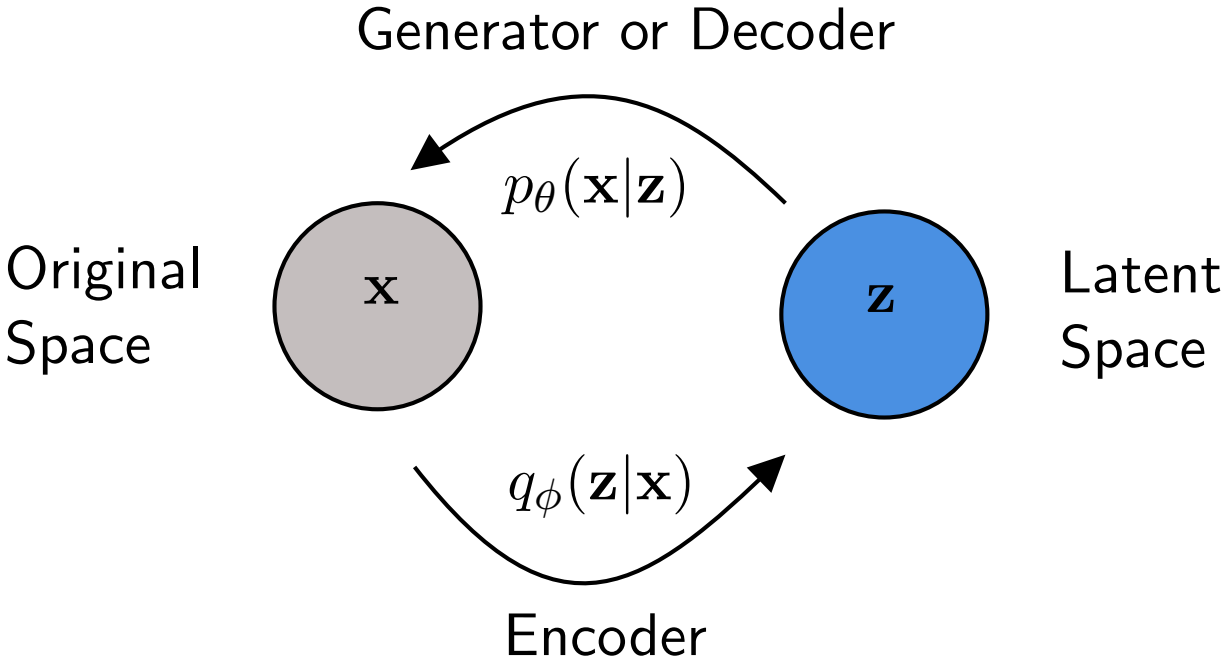
Assume we would like to compute the likelihood of an image $\mathbf{x}$ from the training set:

$$
\begin{aligned}
\mathcal{L}(\mathbf{x}) &= \log(p(\mathbf{x})) \\
&= \sum_z q(z|\mathbf{x}) \log(p(\mathbf{x})) \\
&= \sum_z q(z|\mathbf{x}) \log\left(\frac{p(z,\mathbf{x})}{p(z|\mathbf{x})}\right) \\
&= \sum_z q(z|\mathbf{x}) \log\left(\frac{p(z,\mathbf{x})q(z|\mathbf{x})}{q(z|\mathbf{x})p(z|\mathbf{x})}\right) \\
&= \sum_z q(z|\mathbf{x}) \log\left(\frac{p(z,\mathbf{x})}{q(z|\mathbf{x})}\right) + \sum_z q(z|\mathbf{x}) \log\left(\frac{q(z|\mathbf{x})}{p(z|\mathbf{x})}\right) \\
&= \sum_z q(z|\mathbf{x}) \log\left(\frac{p(z,\mathbf{x})}{q(z|\mathbf{x})}\right) + \underbrace{D_{KL}(q(z|\mathbf{x}), p(z|\mathbf{x}))}_{\geq 0} \\
&= \mathcal{L}^{lvb}(\mathbf{x}) + D_{KL}(q(z|\mathbf{x}), p(z|\mathbf{x})) \\
&\geq \mathcal{L}^{lvb}(\mathbf{x})
\end{aligned}
$$

$$
\begin{aligned}
\mathcal{L}(\mathbf{x}) \geq \mathcal{L}^{lvb}(\mathbf{x}) &= \sum_z q(z|\mathbf{x}) \log\left(\frac{p(z,\mathbf{x})}{q(z|\mathbf{x})}\right) \\
&= \sum_z q(z|\mathbf{x}) \log\left(\frac{p(\mathbf{x}|z)p(z)}{q(z|\mathbf{x})}\right) \\
&= \sum_z q(z|\mathbf{x}) \log(p(\mathbf{x}|z)) + \sum_z q(z|\mathbf{x}) \log\left(\frac{p(z)}{q(z|\mathbf{x})}\right) \\
&= \mathbb{E}_{q(z|\mathbf{x})} \log(p(\mathbf{x}|z)) - D_{KL}(q(z|\mathbf{x}), p(z)) \\
&= \underbrace{\mathbb{E}_{q(z|\mathbf{x})} \log(p(\mathbf{x}|z))}_{\texttt{Expected Reconstruction}} - \underbrace{D_{KL}(q(z|\mathbf{x}), p(z))}_{\texttt{Regularization } \mathcal{N}(0,1)}
\end{aligned}
$$

- First term implies the use of many realization of sampling process (in practice we only have a few of samples per training example!)
- Second term is simply a formula for diagonal multivariate Gaussian distribution.

Variational Framework



- The $q(\mathbf{z}|\mathbf{x})$ defines a distribution over the latent space $\mathbf{z}$ for the observations $\mathbf{x}$
- The $p(\mathbf{x}|\mathbf{z})$ defines a distribution over the original by decoding latent variable into the observations space.
- ϕ, θ denote parameters to be learned.
- The generation is performed by taking a point in the latent space and applying the decoder.

Latent variable intuition

We can imagine the latent variables and data we observed as modelled by joint distribution $p(\mathbf{x}, \mathbf{z})$
One approach of generative modelling, called *likelihood-based*, is to learn a model to maximise the likelihood $p(\mathbf{x})$ of all observed $\mathbf{x}$

1. Marginalize: $p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{z}) d\mathbf{z}$
2. Chain rule of probability: $p(\mathbf{x}) = \frac{p(\mathbf{x}, \mathbf{z})}{p(\mathbf{z}|\mathbf{x})}$

Latent variable intuition

We can imagine the latent variables and data we observed as modelled by joint distribution $p(\mathbf{x}, \mathbf{z})$
One approach of generative modelling, called *likelihood-based*, is to learn a model to maximise the likelihood $p(\mathbf{x})$ of all observed $\mathbf{x}$

1. Marginalize: $p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{z}) d\mathbf{z}$
2. Chain rule of probability: $p(\mathbf{x}) = \frac{p(\mathbf{x}, \mathbf{z})}{p(\mathbf{z}|\mathbf{x})}$

The main difficulties of:
(1) is that it involves integrating out all latent variables $\mathbf{z}$, which is intractable for complex models.
(2) is that it involves having access to $p(\mathbf{z}|\mathbf{x})$, the truth latent encoder.

Latent variable intuition

We can imagine the latent variables and data we observed as modelled by joint distribution $p(\mathbf{x}, \mathbf{z})$
One approach of generative modelling, called *likelihood-based*, is to learn a model to maximise the likelihood $p(\mathbf{x})$ of all observed $\mathbf{x}$

1. Marginalize: $p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{z}) d\mathbf{z}$
2. Chain rule of probability: $p(\mathbf{x}) = \frac{p(\mathbf{x},\mathbf{z})}{p(\mathbf{z}|\mathbf{x})}$

The main difficulties of:
(1) is that it involves integrating out all latent variables $\mathbf{z}$, which is intractable for complex models.
(2) is that it involves having access to $p(\mathbf{z}|\mathbf{x})$, the truth latent encoder. Solution: Find a lower bound of the log likelihood of the observed data (called the *Evidence Lower Bound*, ELBO)

ELBO derivation

$$\log p(\mathbf{x}) \quad = \quad \log p(\mathbf{x})$$

ELBO derivation

$$
\begin{aligned}
\log p(\mathbf{x}) &= \log p(\mathbf{x}) \\
&= \log p(\mathbf{x}) \int q_\phi(\mathbf{z}|\mathbf{x}) d\mathbf{z} \quad \texttt{(Multiplying by 1)}
\end{aligned}
$$

ELBO derivation

$$
\begin{aligned}
\log p(\mathbf{x}) &= \log p(\mathbf{x}) \\
&= \log p(\mathbf{x}) \int q_\phi(\mathbf{z}|\mathbf{x}) d\mathbf{z} \quad (\texttt{Multiplying by 1}) \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}(\log p(\mathbf{x})) \quad (\texttt{Def. Expected value})
\end{aligned}
$$

ELBO derivation

$$
\begin{aligned}
\log p(\mathbf{x}) &= \log p(\mathbf{x}) \\
&= \log p(\mathbf{x}) \int q_\phi(\mathbf{z}|\mathbf{x}) d\mathbf{z} \quad (\texttt{Multiplying by 1}) \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}(\log p(\mathbf{x})) \quad (\texttt{Def. Expected value}) \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left(\log \frac{p(\mathbf{x},\mathbf{z})}{p(\mathbf{z}|\mathbf{x})}\right) \quad (\texttt{Chain Rule of probability})
\end{aligned}
$$

ELBO derivation

$$
\begin{aligned}
\log p(\mathbf{x}) &= \log p(\mathbf{x}) \\
&= \log p(\mathbf{x}) \int q_\phi(\mathbf{z}|\mathbf{x}) d\mathbf{z} \quad (\texttt{Multiplying by 1}) \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}(\log p(\mathbf{x})) \quad (\texttt{Def. Expected value}) \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left(\log \frac{p(\mathbf{x},\mathbf{z})}{p(\mathbf{z}|\mathbf{x})}\right) \quad (\texttt{Chain Rule of probability}) \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left(\log \frac{p(\mathbf{x},\mathbf{z}) q_\phi(\mathbf{z}|\mathbf{x})}{p(\mathbf{z}|\mathbf{x}) q_\phi(\mathbf{z}|\mathbf{x})}\right)
\end{aligned}
$$

ELBO derivation

$$
\begin{aligned}
\log p(\mathbf{x}) &= \log p(\mathbf{x}) \\
&= \log p(\mathbf{x}) \int q_\phi(\mathbf{z}|\mathbf{x}) d\mathbf{z} \quad \texttt{(Multiplying by 1)} \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}(\log p(\mathbf{x})) \quad \texttt{(Def. Expected value)} \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left(\log \frac{p(\mathbf{x},\mathbf{z})}{p(\mathbf{z}|\mathbf{x})}\right) \quad \texttt{(Chain Rule of probability)} \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left(\log \frac{p(\mathbf{x},\mathbf{z}) q_\phi(\mathbf{z}|\mathbf{x})}{p(\mathbf{z}|\mathbf{x}) q_\phi(\mathbf{z}|\mathbf{x})}\right) \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left(\log \frac{p(\mathbf{x},\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}\right) + \underbrace{\mathbb{E}_{q_{\phi(\mathbf{z}|\mathbf{x})}}\left(\log \frac{q_\phi(\mathbf{z}|\mathbf{x})}{p(\mathbf{z}|\mathbf{x})}\right)}_{\texttt{KL Divergence} \geq 0}
\end{aligned}
$$

ELBO derivation

$$
\begin{aligned}
\log p(\mathbf{x}) &= \log p(\mathbf{x}) \\
&= \log p(\mathbf{x}) \int q_\phi(\mathbf{z}|\mathbf{x}) d\mathbf{z} \quad (\texttt{Multiplying by 1}) \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}(\log p(\mathbf{x})) \quad (\texttt{Def. Expected value}) \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left(\log \frac{p(\mathbf{x},\mathbf{z})}{p(\mathbf{z}|\mathbf{x})}\right) \quad (\texttt{Chain Rule of probability}) \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left(\log \frac{p(\mathbf{x},\mathbf{z}) q_\phi(\mathbf{z}|\mathbf{x})}{p(\mathbf{z}|\mathbf{x}) q_\phi(\mathbf{z}|\mathbf{x})}\right) \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left(\log \frac{p(\mathbf{x},\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}\right) + \underbrace{\mathbb{E}_{q_{\phi(\mathbf{z}|\mathbf{x})}}\left(\log \frac{q_\phi(\mathbf{z}|\mathbf{x})}{p(\mathbf{z}|\mathbf{x})}\right)}_{\texttt{KL Divergence} \geq 0}
\end{aligned}
$$

The KL divergence between the approximate posterior $q_\phi(\mathbf{z}|\mathbf{x})$ and the true posterior $p(\mathbf{z}|\mathbf{x})$.

ELBO derivation

$$
\begin{aligned}
\log p(\mathbf{x}) &= \log p(\mathbf{x}) \\
&= \log p(\mathbf{x}) \int q_{\phi(\mathbf{z}|\mathbf{x})} d\mathbf{z} \quad (\texttt{Multiplying by 1}) \\
&= \mathbb{E}_{q_{\phi(\mathbf{z}|\mathbf{x})}} (\log p(\mathbf{x})) \quad (\texttt{Def. Expected value}) \\
&= \mathbb{E}_{q_{\phi(\mathbf{z}|\mathbf{x})}} \left(\log \frac{p(\mathbf{x}, \mathbf{z})}{p(\mathbf{z}|\mathbf{x})} \right) \quad (\texttt{Chain Rule of probability}) \\
&= \mathbb{E}_{q_{\phi(\mathbf{z}|\mathbf{x})}} \left(\log \frac{p(\mathbf{x}, \mathbf{z}) q_\phi(\mathbf{z}|\mathbf{x})}{p(\mathbf{z}|\mathbf{x}) q_\phi(\mathbf{z}|\mathbf{x})} \right) \\
&= \mathbb{E}_{q_{\phi(\mathbf{z}|\mathbf{x})}} \left(\log \frac{p(\mathbf{x}, \mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})} \right) + \underbrace{\mathbb{E}_{q_{\phi(\mathbf{z}|\mathbf{x})}} \left(\log \frac{q_\phi(\mathbf{z}|\mathbf{x})}{p(\mathbf{z}|\mathbf{x})} \right)}_{\texttt{KL Divergence} \geq 0}
\end{aligned}
$$

ELBO derivation

$$
\begin{aligned}
\log p(\mathbf{x}) &= \log p(\mathbf{x}) \\
&= \log p(\mathbf{x}) \int q_{\phi(\mathbf{z}|\mathbf{x})} d\mathbf{z} \quad \texttt{(Multiplying by 1)} \\
&= \mathbb{E}_{q_{\phi(\mathbf{z}|\mathbf{x})}} (\log p(\mathbf{x})) \quad \texttt{(Def. Expected value)} \\
&= \mathbb{E}_{q_{\phi(\mathbf{z}|\mathbf{x})}} \left(\log \frac{p(\mathbf{x}, \mathbf{z})}{p(\mathbf{z}|\mathbf{x})} \right) \quad \texttt{(Chain Rule of probability)} \\
&= \mathbb{E}_{q_{\phi(\mathbf{z}|\mathbf{x})}} \left(\log \frac{p(\mathbf{x}, \mathbf{z}) q_\phi(\mathbf{z}|\mathbf{x})}{p(\mathbf{z}|\mathbf{x}) q_\phi(\mathbf{z}|\mathbf{x})} \right) \\
&= \mathbb{E}_{q_{\phi(\mathbf{z}|\mathbf{x})}} \left(\log \frac{p(\mathbf{x}, \mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})} \right) + \underbrace{\mathbb{E}_{q_{\phi(\mathbf{z}|\mathbf{x})}} \left(\log \frac{q_\phi(\mathbf{z}|\mathbf{x})}{p(\mathbf{z}|\mathbf{x})} \right)}_{\texttt{KL Divergence} \geq 0} \\
&\geq \mathbb{E}_{q_{\phi(\mathbf{z}|\mathbf{x})}} \left(\log \frac{p(\mathbf{x}, \mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})} \right)
\end{aligned}
$$

The KL divergence between the approximate posterior $q_\phi(\mathbf{z}|\mathbf{x})$ and the true posterior $p(\mathbf{z}|\mathbf{x})$.

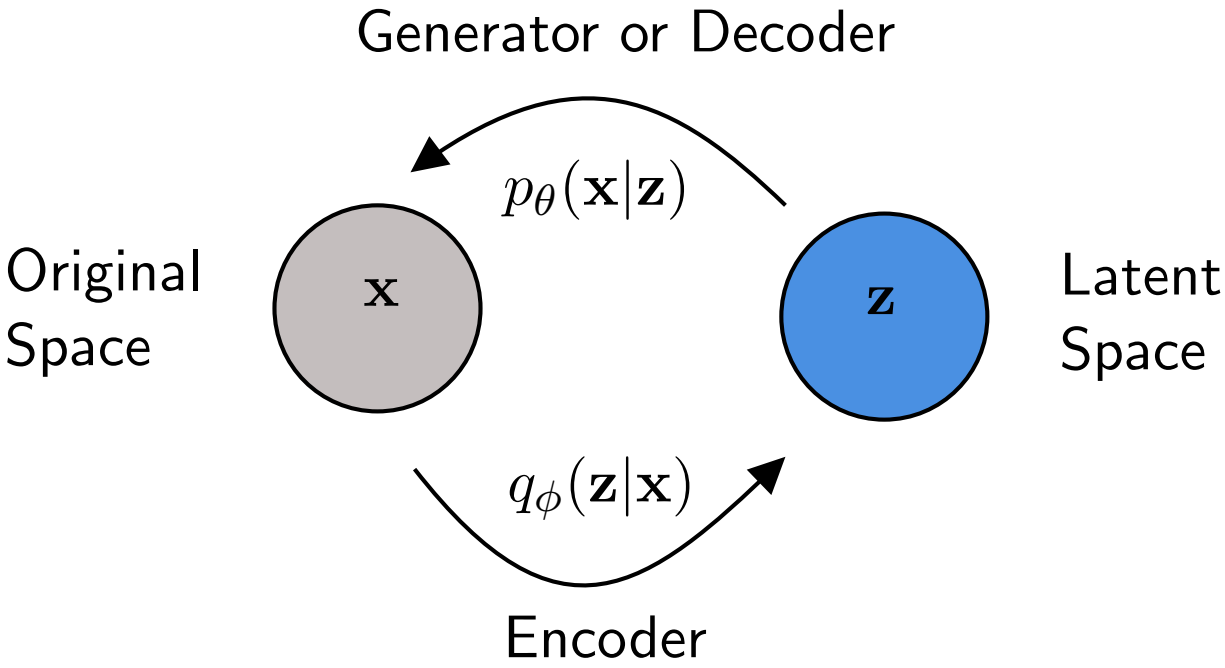
Evidence Lower Bound (ELBO)

The goal is maximise the

$$\log p(\mathbf{x}) \geq \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left(\log \frac{p(\mathbf{x},\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}\right)$$

$$\begin{aligned}
\log p(\mathbf{x}) &\geq \mathbb{E}_{q_{\phi(\mathbf{z}|\mathbf{x})}}\left(\log \frac{p(\mathbf{x},\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}\right) \\
&= \mathbb{E}_{q_{\phi(\mathbf{z}|\mathbf{x})}}\left(\log \frac{p_\theta(\mathbf{x}|\mathbf{z})p(\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}\right) \\
&= \underbrace{\mathbb{E}_{q_{\phi(\mathbf{z}|\mathbf{x})}}[\log p_\theta(\mathbf{x}|\mathbf{z})]}_{\texttt{Reconstruction term}} - \underbrace{\mathbb{E}_{q_{\phi(\mathbf{z}|\mathbf{x})}}\left(\log \frac{p(\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}\right)}_{\texttt{KL Divergence}\geq 0}
\end{aligned}$$

The KL divergence between the approximate posterior $q_\phi(\mathbf{z}|\mathbf{x})$ and a prior term $p(\mathbf{z})$, usually considered as Gaussian Distribution.


Generator or Decoder
$p_\theta(\mathbf{x}|\mathbf{z})$
Original Space
$\mathbf{x}$
$\mathbf{z}$
Latent Space
$q_\phi(\mathbf{z}|\mathbf{x})$
Encoder

Interpretation

1. The first term measures the reconstruction likelihood of the decoder. Ensure that the learned distribution models effective the problem.
2. The second term gives a priori belief of variables on latent space. Minimising this term encourage the encoder to learn the prior distribution instead of collapse into a point (Dirac delta function).

Contents

1. Introduction
2. Generative models
   - Classical Generative Modeling
   - Autoencoders
   - Variational Autoencoder
3. Generative Adversarial Networks (GANs)
4. Variational Diffusion Models
5. References

Contents

1. Introduction
2. Generative models
3. Generative Adversarial Networks (GANs)
4. Variational Diffusion Models
5. References

Generative Adversarial Networks (GANs)

We require that the discriminator D recognises examples from the $P_{\texttt{real}}(\mathbf{x})$ distribution,

$$\mathbb{E}_{\mathbf{x}\sim P_{\texttt{real}}(\mathbf{x})}[\log D(\mathbf{x})] \qquad \texttt{Decision over Real Data}$$

where $\mathbb{E}$ denotes the expectation. This term comes from the "1" class of the log-loss function.
Additionally, we would like to trick the discriminator via a good generator G. Thus, the term comes from "0" class of the log-loss function:

$$\mathbb{E}_{z\sim P_z(z)}[\log(1 - D(G(z)))] \qquad \texttt{Decision over Fake Data}$$

Generative Adversarial Networks (GANs)

Questions: Optimal Discriminator? Optimal Generator? We define:

$$V(G, D) := \mathbb{E}_{\mathbf{x} \sim P_{\texttt{real}}(\mathbf{x})}[\log D(\mathbf{x})] + \mathbb{E}_{z \sim P_z(z)}[\log(1 - D(G(z)))]$$

What should be an optimal discriminator?

Generative Adversarial Networks (GANs)

Questions: Optimal Discriminator? Optimal Generator? We define:

$$V(G, D) := \mathbb{E}_{\mathbf{x} \sim P_{\texttt{real}}(\mathbf{x})}[\log D(\mathbf{x})] + \mathbb{E}_{z \sim P_z(z)}[\log(1 - D(G(z)))]$$

What should be an optimal discriminator?

$$D^* = \arg\max_D V(G, D)$$

Now, given this optimal discriminator D^*, what should be an optimal generator?

Generative Adversarial Networks (GANs)

Questions: Optimal Discriminator? Optimal Generator? We define:

$$V(G, D) := \mathbb{E}_{\mathbf{x} \sim P_{\texttt{real}}(\mathbf{x})}[\log D(\mathbf{x})] + \mathbb{E}_{z \sim P_z(z)}[\log(1 - D(G(z)))]$$

What should be an optimal discriminator?

$$D^* = \arg\max_D V(G, D)$$

Now, given this optimal discriminator D^*, what should be an optimal generator?

$$G^* = \arg\min_G V(G, D^*)$$

This is called the *minimax formulation*, since the generator and discriminator are playing a *zero-sum game* against each other:

$$\min_G \max_D V(G, D) \tag{3}$$

Generative Adversarial Networks (GANs)

$$
\begin{aligned}
& \min_G \max_D V(G,D) := \\
= \quad & \mathbb{E}_{\mathbf{x}\sim P_{\texttt{real}}(\mathbf{x})}[\log D(\mathbf{x})] + \mathbb{E}_{z\sim P_z(z)}[\log(1-D(G(z)))] \\
& \texttt{by Radon-Nikodym Theorem} \\
= \quad & \mathbb{E}_{\mathbf{x}\sim P_{\texttt{real}}(\mathbf{x})}[\log D(\mathbf{x})] + \mathbb{E}_{x\sim P_{g(\mathbf{x})}}[\log(1-D(x))] \\
= \quad & \int_x \left(P_{\texttt{real}}(\mathbf{x})[\log D(\mathbf{x})] + P_{g(\mathbf{x})}[\log(1-D(x))] \right) dx
\end{aligned}
$$

$$V(G,D) = \int_x \left(P_{\texttt{real}}(\mathbf{x})[\log D(\mathbf{x})] + P_{g(\mathbf{x})}[\log(1 - D(x))] \right) dx \tag{4}$$

- Note that $f(x) = a\log(x) + b\log(1-x)$, has minimum in $x^* = \frac{a}{a+b}$

$$V(G,D) = \int_x \left(P_{\texttt{real}}(\mathbf{x})[\log D(\mathbf{x})] + P_{g(\mathbf{x})}[\log(1 - D(x))] \right) dx \tag{4}$$

- Note that $f(x) = a\log(x) + b\log(1-x)$, has minimum in $x^* = \frac{a}{a+b}$
- Then If G is fixed,
- $P_{\texttt{real}}(\mathbf{x}) \log D(\mathbf{x}) + P_{g(\mathbf{x})} \log(1 - D(x))$ the optimal discriminator $D^*(\mathbf{x}) = \frac{P_{\texttt{real}}(\mathbf{x})}{P_{\texttt{real}}(\mathbf{x}) + P_{\texttt{g}}(\mathbf{x})}$

Given an optimal discriminator $D^*(\mathbf{x})$, find $\min_G V(G, D^*)$.

$$\int_x (P_{\texttt{real}}(\mathbf{x}) \log\left(\frac{P_{\texttt{real}}(\mathbf{x})}{P_{\texttt{real}}(\mathbf{x}) + P_{\texttt{g}}(\mathbf{x})}\right) + P_{g(\mathbf{x})} \log\left(1 - \frac{P_{\texttt{real}}(\mathbf{x})}{P_{\texttt{real}}(\mathbf{x}) + P_{\texttt{g}}(\mathbf{x})}\right)$$

[1]Divergence Jensen–Shannon is a symmetrized and smoothed version of the Kullback–Leibler divergence, $Div_{\texttt{JS}}(p||q) = \frac{1}{2} Div_{\texttt{KL}}(p||m) + \frac{1}{2} Div_{\texttt{KL}}(q||m)$ where $m = p + q$

Given an optimal discriminator $D^*(\mathbf{x})$, find $\min_G V(G, D^*)$.

$$\int_x (P_{\texttt{real}}(\mathbf{x}) \log\left(\frac{P_{\texttt{real}}(\mathbf{x})}{P_{\texttt{real}}(\mathbf{x}) + P_{\texttt{g}}(\mathbf{x})}\right) + P_{g(\mathbf{x})} \log\left(1 - \frac{P_{\texttt{real}}(\mathbf{x})}{P_{\texttt{real}}(\mathbf{x}) + P_{\texttt{g}}(\mathbf{x})}\right)$$

by means of Divergence Jensen–Shannon[1] we can obtain:

$$Div_{\texttt{JS}}(P_{\texttt{real}} || P_{\texttt{g}}) = \frac{1}{2}(\log 4 + \min_G V(G, D^*)) \tag{5}$$

[1] Divergence Jensen–Shannon is a symmetrized and smoothed version of the Kullback–Leibler divergence, $Div_{\texttt{JS}}(p||q) = \frac{1}{2} Div_{\texttt{KL}}(p||m) + \frac{1}{2} Div_{\texttt{KL}}(q||m)$ where $m = p + q$

Summarising, we have:

- Optimal Discriminator: $D^*(\mathbf{x}) = \frac{P_{\texttt{real}}(\mathbf{x})}{P_{\texttt{real}}(\mathbf{x}) + P_{\texttt{g}}(\mathbf{x})}$
- $\min_G V(G, D^*) = 2Div_{\texttt{JS}}(P_{\texttt{real}} || P_{\texttt{g}}) - 2\log 2$

Summarising, we have:

- Optimal Discriminator: $D^*(\mathbf{x}) = \frac{P_{\texttt{real}}(\mathbf{x})}{P_{\texttt{real}}(\mathbf{x}) + P_{\texttt{g}}(\mathbf{x})}$
- $\min_G V(G, D^*) = 2Div_{\texttt{JS}}(P_{\texttt{real}} || P_{\texttt{g}}) - 2\log 2$

Thus,

- $\min_G V(G, D^*)$ is obtained when $P_{\texttt{real}} = P_{\texttt{g}}$,

Summarising, we have:

- Optimal Discriminator: $D^*(\mathbf{x}) = \frac{P_{\texttt{real}}(\mathbf{x})}{P_{\texttt{real}}(\mathbf{x}) + P_{\texttt{g}}(\mathbf{x})}$
- $\min_G V(G, D^*) = 2Div_{\texttt{JS}}(P_{\texttt{real}} || P_{\texttt{g}}) - 2\log 2$

Thus,

- $\min_G V(G, D^*)$ is obtained when $P_{\texttt{real}} = P_{\texttt{g}}$,
- $D^*(\mathbf{x}) = \frac{1}{2}$

Summarising, we have:

- Optimal Discriminator: $D^*(\mathbf{x}) = \frac{P_{\texttt{real}}(\mathbf{x})}{P_{\texttt{real}}(\mathbf{x}) + P_{\texttt{g}}(\mathbf{x})}$
- $\min_G V(G, D^*) = 2Div_{\texttt{JS}}(P_{\texttt{real}} || P_{\texttt{g}}) - 2\log 2$

Thus,

- $\min_G V(G, D^*)$ is obtained when $P_{\texttt{real}} = P_{\texttt{g}}$,
- $D^*(\mathbf{x}) = \frac{1}{2}$
- and $\min_G \max_D V(G, D) = -2\log 2$

Proof with more details

1. Annotated Proof of GANs `https://srome.github.io/An-Annotated-Proof-of-Generative-Adversarial-Networks-`
2. Generative Adversarial Nets: (`https://arxiv.org/pdf/1406.2661.pdf`)

Training GANs: Training the Discriminator:

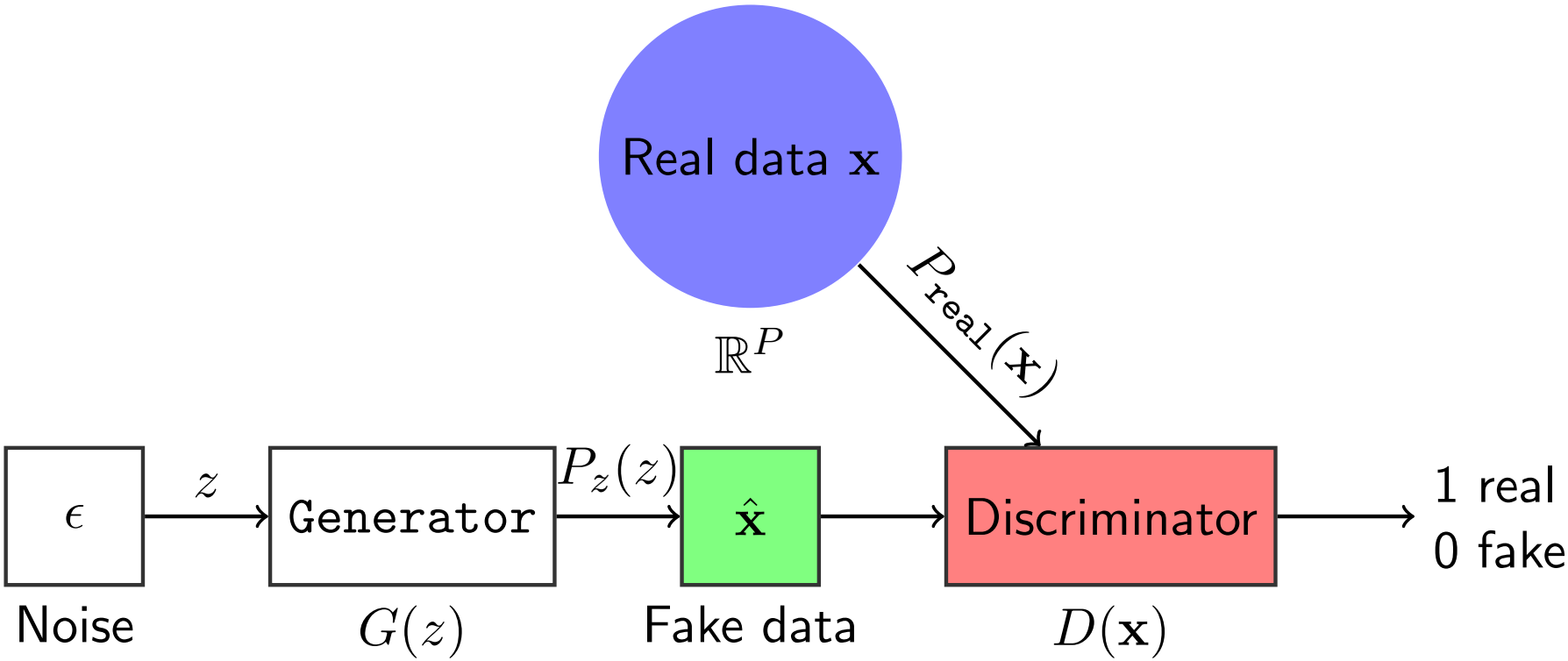


Figure: Only Discriminator should be updated

Training GANs: Training the Generator

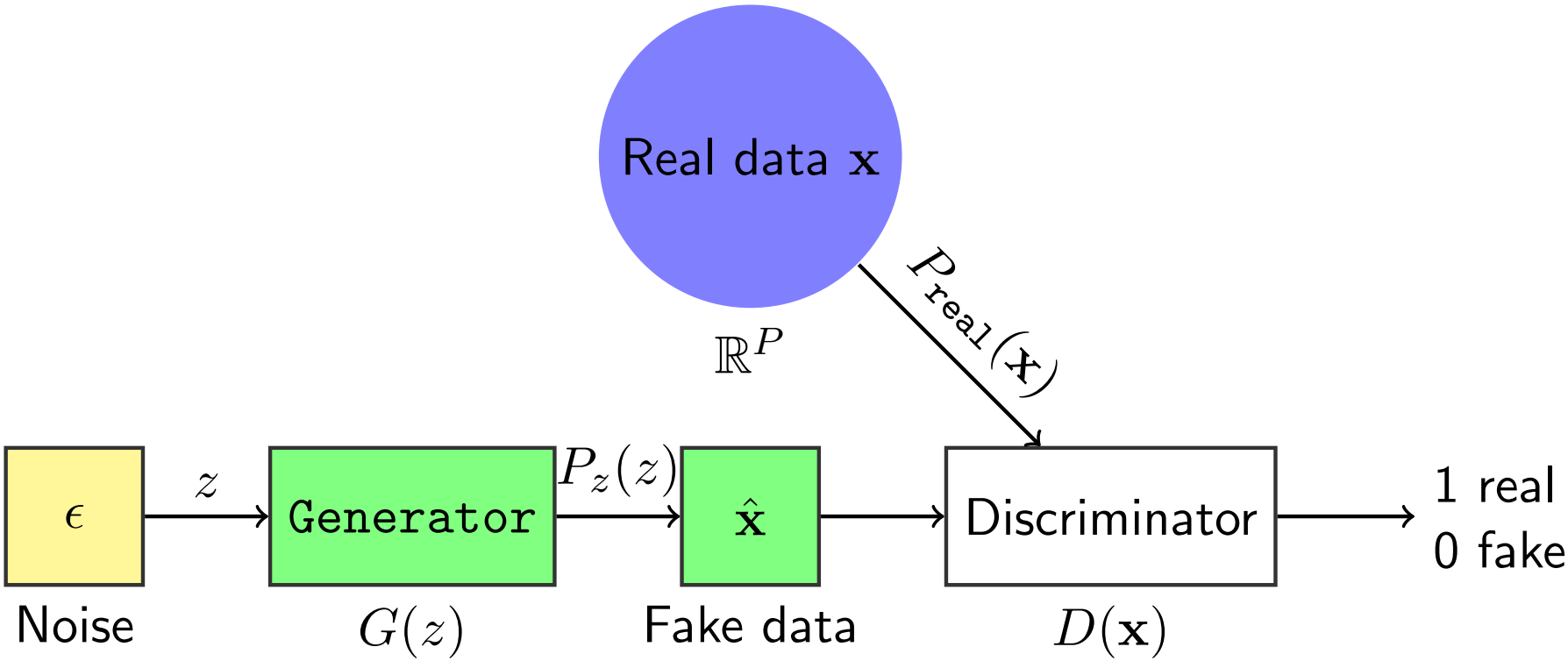


Figure: Discriminator should be set to "non-trainable" weights

How to Train a GAN?

Bad news: GANs are hard to train. **Tips and tricks to make GANs work** `https://github.com/soumith/ganhacks`

- Use others loss functions.
- Avoid Sparse Gradients: ReLU, MaxPool
- Use Deep Convolutional Generative Adversarial Networks when you can. It works!
- Use SGD for discriminator and ADAM for generator
- Use Dropouts in G in both train and test phase
- ...

"In theory, there is no difference between theory and practice. In practice, there is."

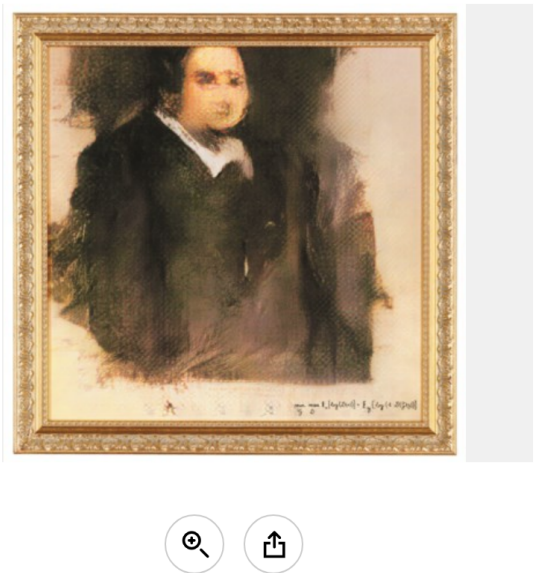
High-resolution GANs

Progressive Growing of GANs for Improved Quality, Stability, and Variation [Karras et al., 2017]
`https://www.youtube.com/watch?v=G06dEcZ-QTg`

Applications of GANs: Earn money!

Applications of GANs: Earn money!

23-25 Oct, 2018: Auction house "Christies" sold a portrait for 432,000 dollars that had been generated by a GANs



LOT 363

Edmond de Belamy, from La Famille de Belamy

Price realised
USD 432,500

Estimate
USD 7,000 - USD 10,000

Follow lot

+ Add to Interests

Edmond de Belamy, from *La Famille de Belamy*
generative Adversarial Network print, on canvas, 2018, signed with GAN model loss function in ink by the publisher, from a series of eleven unique images, published by Obvious Art, Paris, with original gilded wood frame
S. 27 ½ x 27 ½ in (700 x 700 mm.)

GANs to improve simulations

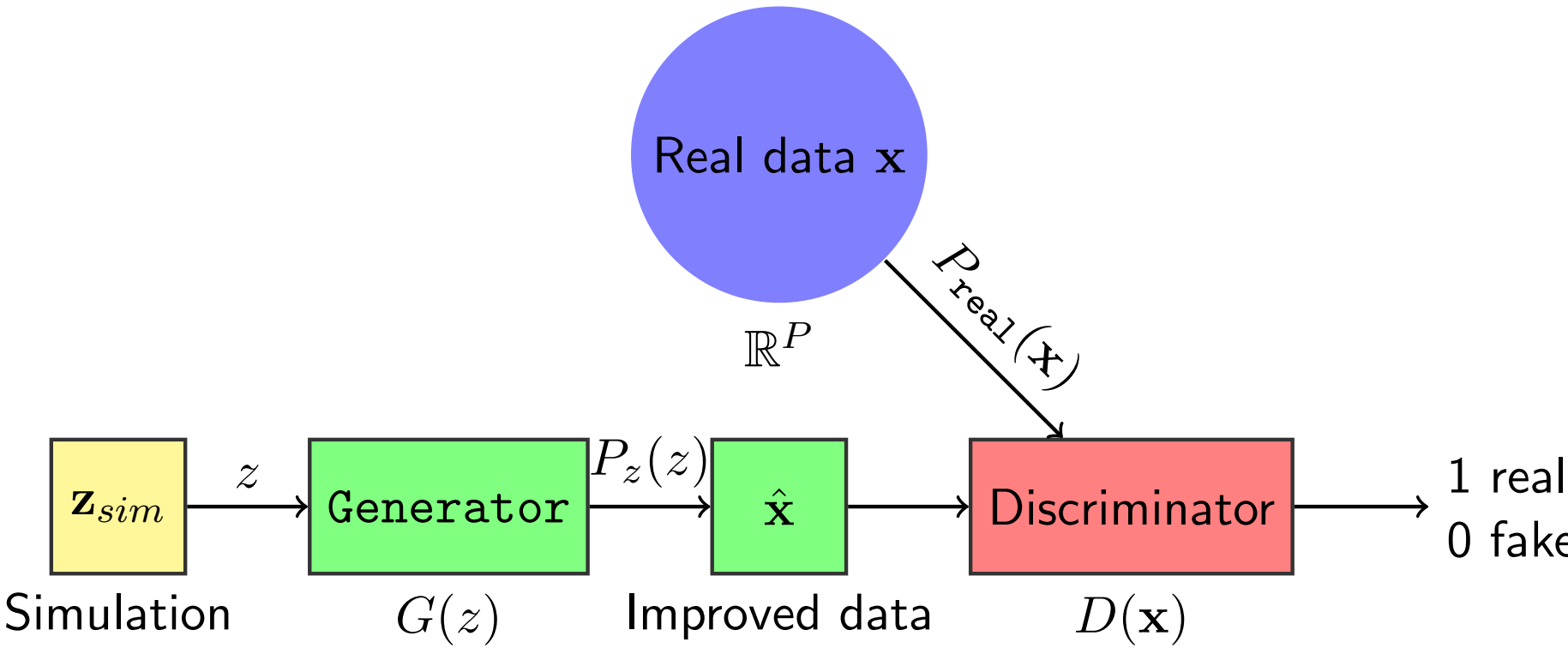


Figure: In this case, `Generator` is called `Refiner`

Application: Refine simulations

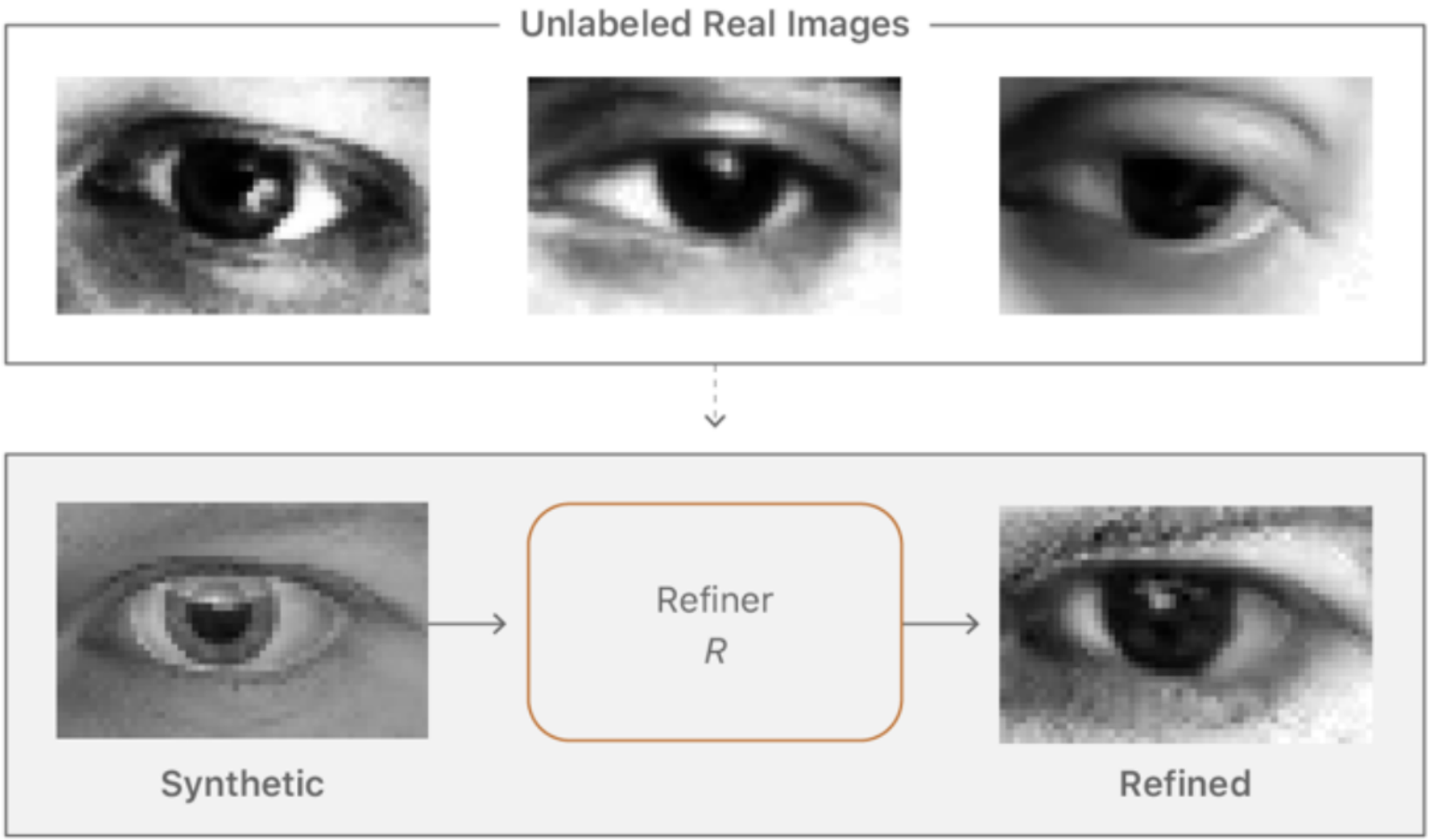
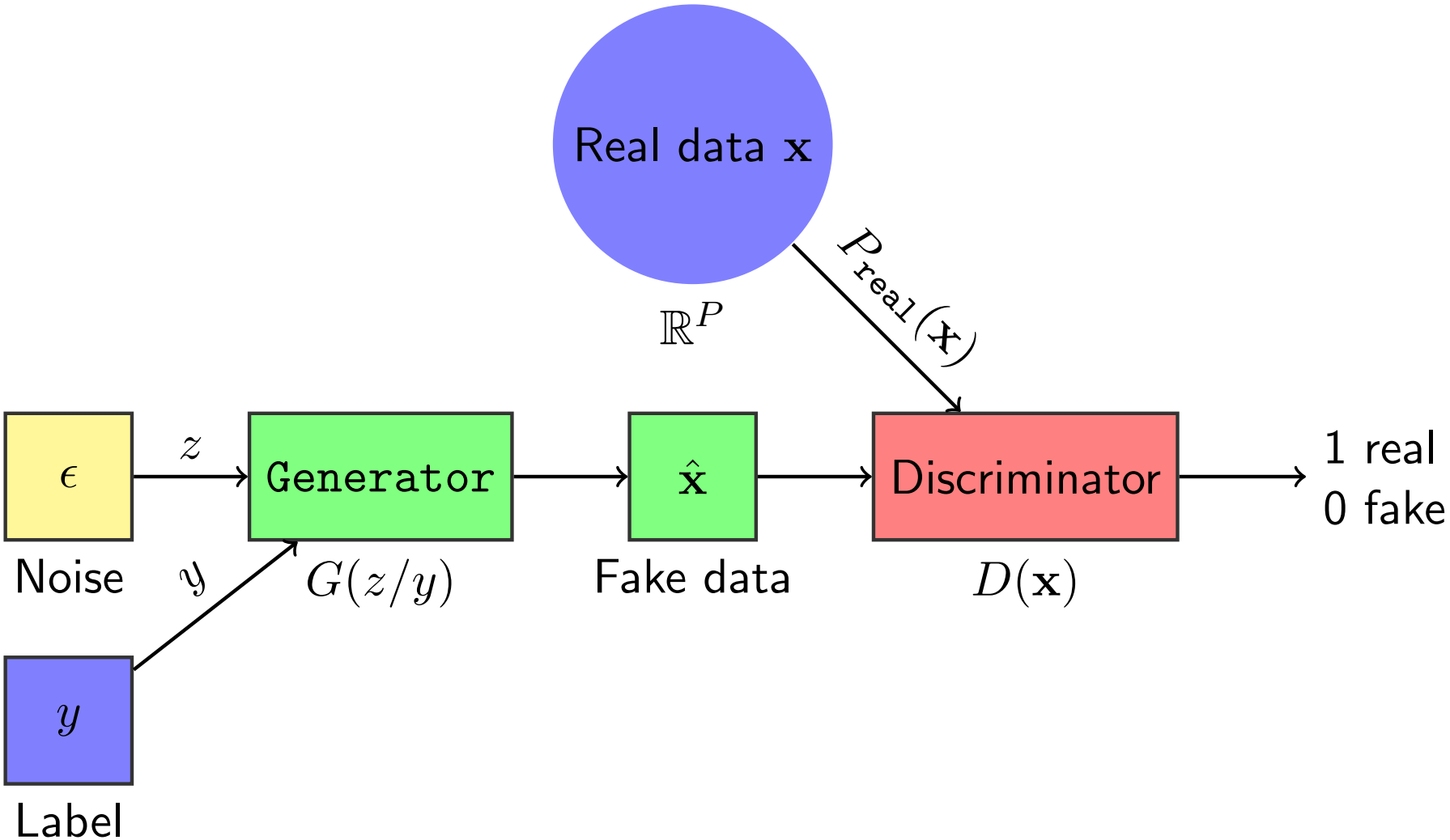


Figure: Learning from Simulated and Unsupervised Images through Adversarial Training [Shrivastava et al., 2017]

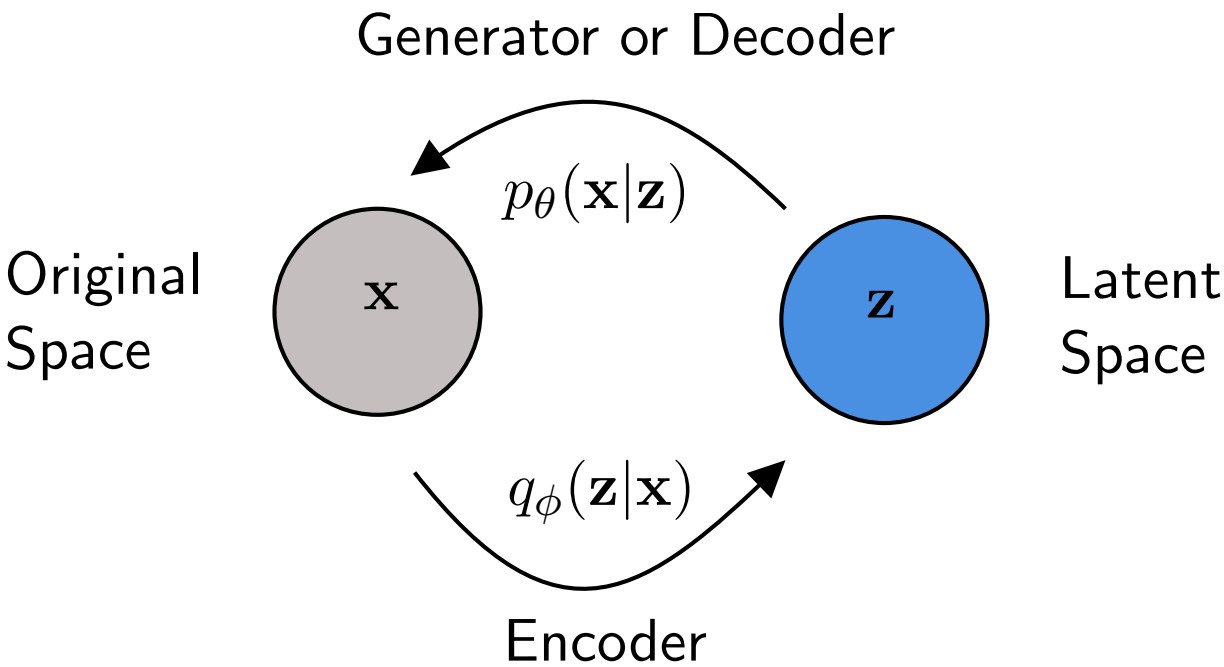
Conditional Generative Adversarial Networks (cGANs)



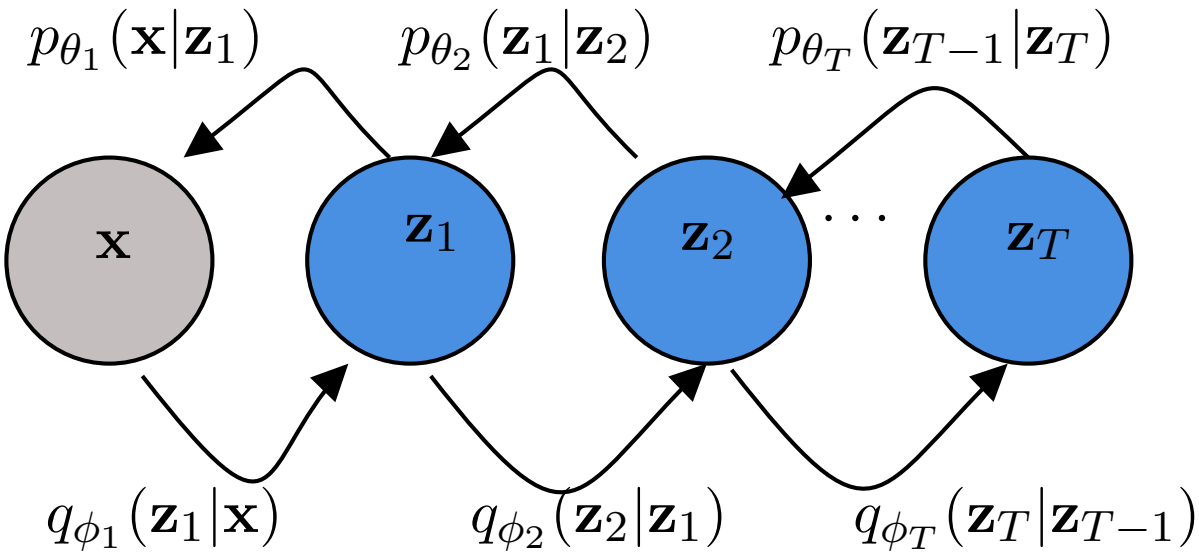
Contents

1. Introduction
2. Generative models
3. Generative Adversarial Networks (GANs)
4. Variational Diffusion Models
5. References

Variational Autoencoder



Markovian variational autoencoder with T hierarchical latent spaces



The generative process is modeled as a Markov Chain, where each latent value $\mathbf{z}_t$ is generated only from he previous latent $\mathbf{z}_{t+1}$.

Markovian variational autoencoder with T hierarchical latent spaces

The joint distribution and the posterior of a Markovian Hierarchical VAE as:

$$p(\mathbf{x}, \mathbf{z}_{1:T}) = p(\mathbf{z}_T) p_{\theta_1}(\mathbf{x}|\mathbf{z}_1) \prod_{t=2}^{T} p_{\theta_t}(\mathbf{z}_{t-1}|\mathbf{z}_t), \tag{6}$$

$$q_\phi(\mathbf{z}_{1:T}|\mathbf{x}) = q_{\phi_1}(\mathbf{z}_1|\mathbf{x}) \prod_{t=2}^{T} q_{\phi_t}(\mathbf{z}_t|\mathbf{z}_{t-1}) \tag{7}$$

ELBO derivation

$$
\begin{aligned}
\log p(\mathbf{x}) &= \log \int p(\mathbf{x}, \mathbf{z}_{1:T}) d\mathbf{z}_{1:T} && (8)\\
&= \log \int \frac{p(\mathbf{x}, \mathbf{z}_{1:T}) q_\phi(\mathbf{z}_{1:T}|\mathbf{x})}{q_\phi(\mathbf{z}_{1:T}|\mathbf{x})} d\mathbf{z}_{1:T} && (9)\\
&= \log \mathbb{E}_{q_\phi(\mathbf{z}_{1:T}|\mathbf{x})} \left(\frac{p(\mathbf{x}, \mathbf{z}_{1:T})}{q_\phi(\mathbf{z}_{1:T}|\mathbf{x})} \right) && (10)\\
&\geq \mathbb{E}_{q_\phi(\mathbf{z}_{1:T}|\mathbf{x})} \log \left(\frac{p(\mathbf{x}, \mathbf{z}_{1:T})}{q_\phi(\mathbf{z}_{1:T}|\mathbf{x})} \right) && (11)
\end{aligned}
$$

Variational Diffusion Models

That is a Markovian variational autoencoder with the following restrictions:

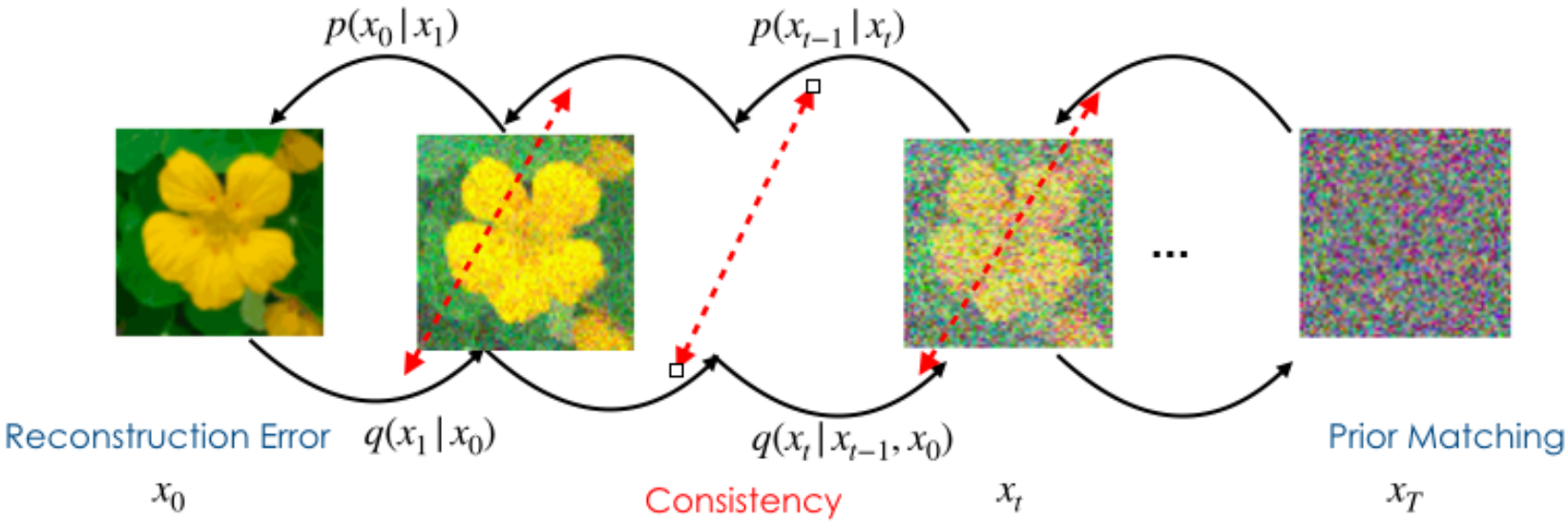
1. The latent dimension is exactly equal to the data dimension
2. The latent encoder at each timestep is predefined as a linear Gaussian model. A Gaussian distribution centred around the output of the previous timestep.
3. After the final timestep T the distribution in the latent space is a standard Gaussian distribution.

Use double conditioning.

$$q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{x}_0) \tag{12}$$

$$\begin{aligned}
\log p(\mathbf{x}) &\geq \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x})} \log \left(\frac{p(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \right) \\
&= \dots \\
&= \underbrace{\mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}+0)}[\log p_\theta(\mathbf{x}_0|\mathbf{x}_1)]}_{\texttt{Reconstruction term}} - \underbrace{\mathbb{E}_{q(\mathbf{x}_T|\mathbf{x}_0)} \left(\log \frac{p(\mathbf{x}_T)}{q(\mathbf{x}_T|\mathbf{x}_{T-1})} \right)}_{\texttt{KL}\geq 0,\ \texttt{Prior Matching Term}} \\
&+ \sum_{t=1}^{T} \underbrace{\mathbb{E}_{q(\mathbf{x}_{t-1},\mathbf{x}_{t+1}|\mathbf{x}_0)} \left(\log \frac{p_\theta(\mathbf{x}_t|\mathbf{x}_{t+1})}{q(\mathbf{x}_t|\mathbf{x}_{t-1})} \right)}_{\texttt{KL}\geq 0,\ \texttt{Consistency term}}
\end{aligned}$$

Variational Diffusion Models



We must be able to **"undo"** the forward noising process:

- Given a target $\mathbf{x}_0$, you must be able to *reverse* the process of noising to reconstruct x_0.
- This noising process happens in small increments.

At the time-step T, the process should be a *random noise*:

- After iteratively adding noise T times, the result must be independent of the starting point x_0

Forward Diffusion

Let α_t be the noise schedule for $t \in \{0, \ldots, T-1\}$. α_t decreases from 1 to 0 as t increase. We can define a *forward* noising function as the distribution:

$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{\alpha}\mathbf{x}_{t-1}, (1-\alpha_t)\mathbf{I}) \tag{13}$$

Forward Diffusion

Let α_t be the noise schedule for $t \in \{0, \ldots, T-1\}$. α_t decreases from 1 to 0 as t increase. We can define a *forward* noising function as the distribution:

$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{\alpha}\mathbf{x}_{t-1}, (1-\alpha_t)\mathbf{I}) \tag{13}$$

We can also arbitrary sample
$\mathbf{x}_t \sim q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I})$ where $\bar{\alpha}_t = \prod_{i=1}^{t} \alpha_i$

Reverse Diffusion

The "reverse" denoising function as the posterior distribution:

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1}; \frac{1}{1-\bar{\alpha}_t}(\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})\mathbf{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)\mathbf{x}_0) \\ , \frac{(1-\alpha_t)(1-\bar{\alpha}_t)}{1-\bar{\alpha}_{t-1}}\mathbf{I}) \\ = \mathcal{N}(\mathbf{x}_{t-1}; \mu_q(\mathbf{x}_t, \mathbf{x}_0), \Sigma_q(t))$$

We call the reverse diffusion process parameterised by a model

$$p(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \frac{1}{1-\bar{\alpha}_t}(\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1}\mathbf{x}_t) + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)\hat{\mathbf{x}}_0), \\ \frac{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{I})$$

Where the model defines the distribution over $\hat{\mathbf{x}}_0$:

$$p(\hat{\mathbf{x}}_0|\mathbf{x}_t, \mathbf{c}) = \texttt{model}_\theta(\mathbf{x}_t, \mathbf{c})$$

Reverse Diffusion Example

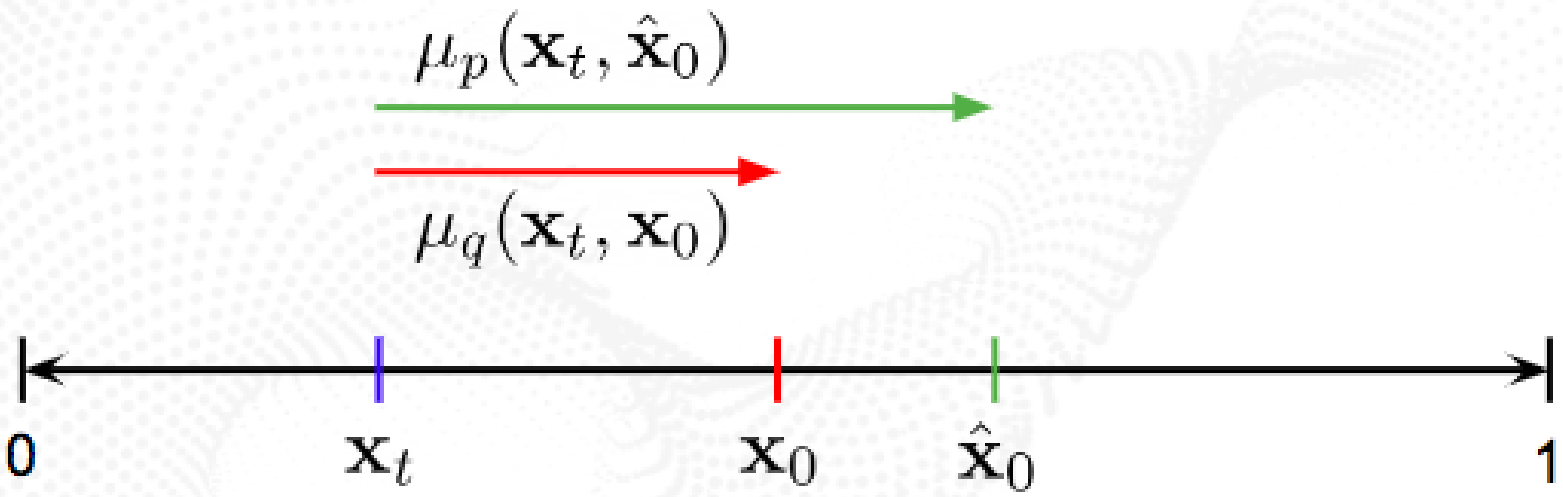
Consider a single pixel of a greyscale image, where the value ranges from 0 to 1

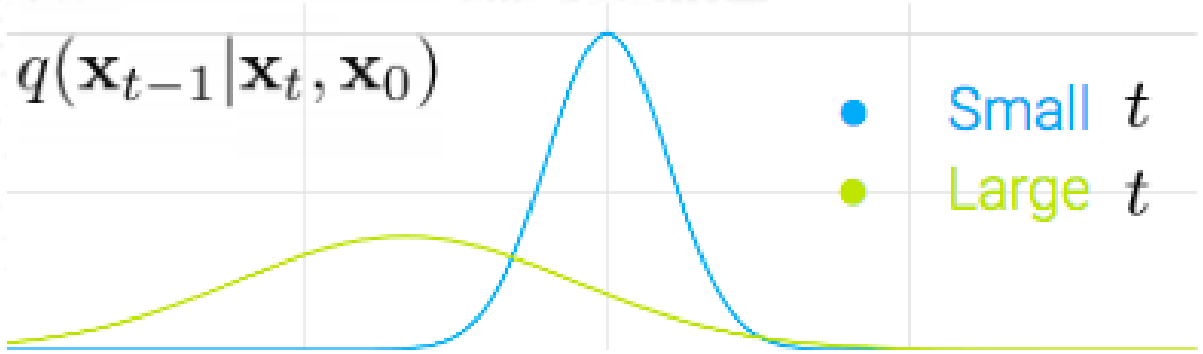
- Current value at $\mathbf{x}_t$
- Target value at $\mathbf{x}_0$
- Model prediction at $\hat{\mathbf{x}}_0$

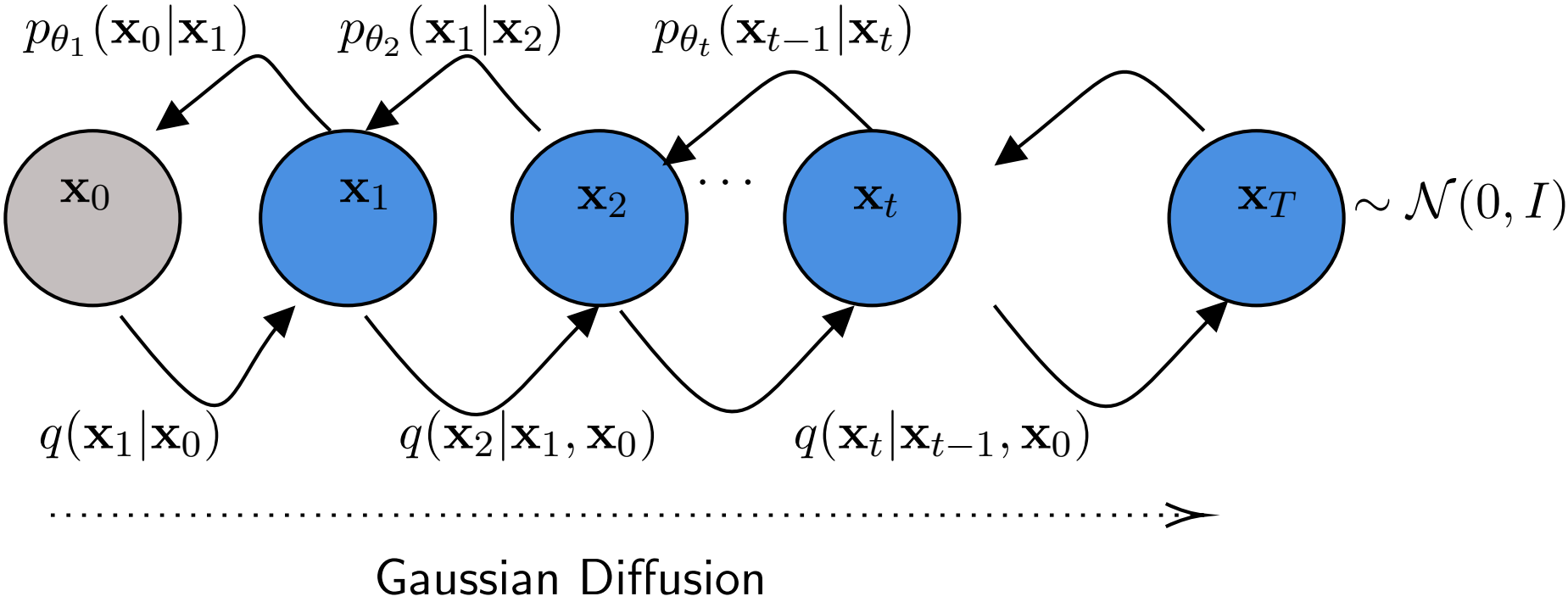
Reverse Diffusion Example

Consider a single pixel of a greyscale image, where the value ranges from 0 to 1

- Current value at $\mathbf{x}_t$
- Target value at $\mathbf{x}_0$
- Model prediction at $\hat{\mathbf{x}}_0$






$p_{\theta_1}(\mathbf{x}_0|\mathbf{x}_1)$
$p_{\theta_2}(\mathbf{x}_1|\mathbf{x}_2)$
$p_{\theta_t}(\mathbf{x}_{t-1}|\mathbf{x}_t)$
$\mathbf{x}_0$
$\mathbf{x}_1$
$\mathbf{x}_2$
$\cdots$
$\mathbf{x}_t$
$\mathbf{x}_T$
$\sim \mathcal{N}(0, I)$
$q(\mathbf{x}_1|\mathbf{x}_0)$
$q(\mathbf{x}_2|\mathbf{x}_1, \mathbf{x}_0)$
$q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{x}_0)$
Gaussian Diffusion

Diffusion models

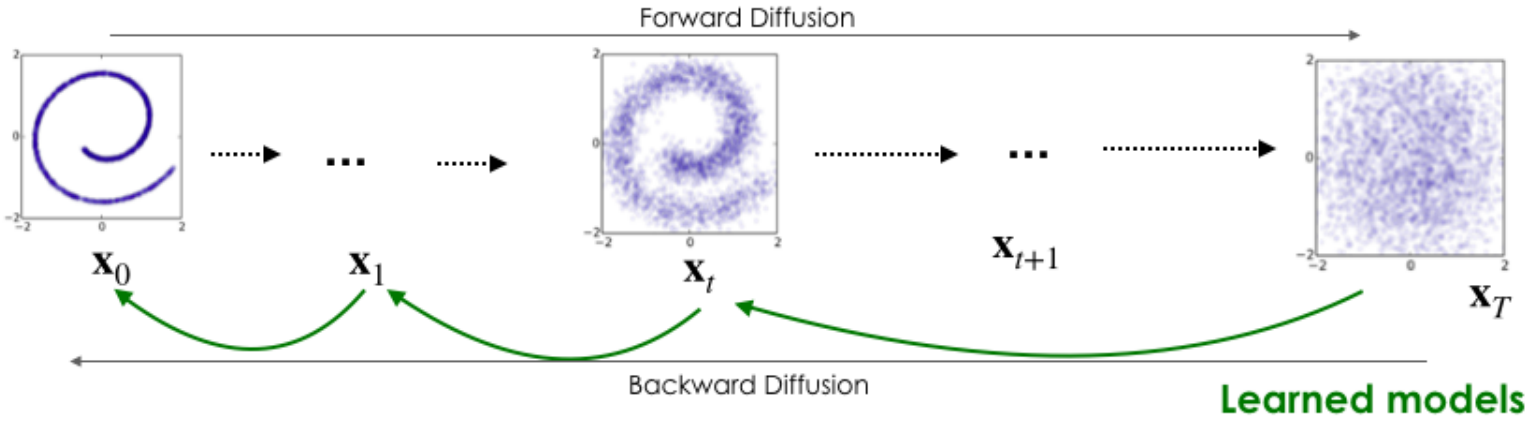


Figure: Diffusion models

Denoising Diffusion models

Over the last two years massive advances in the field of image synthesis with generative models have been made.

1. DALL-E 2
2. Midjourney
3. Stable Diffusion

Stable Diffusion models

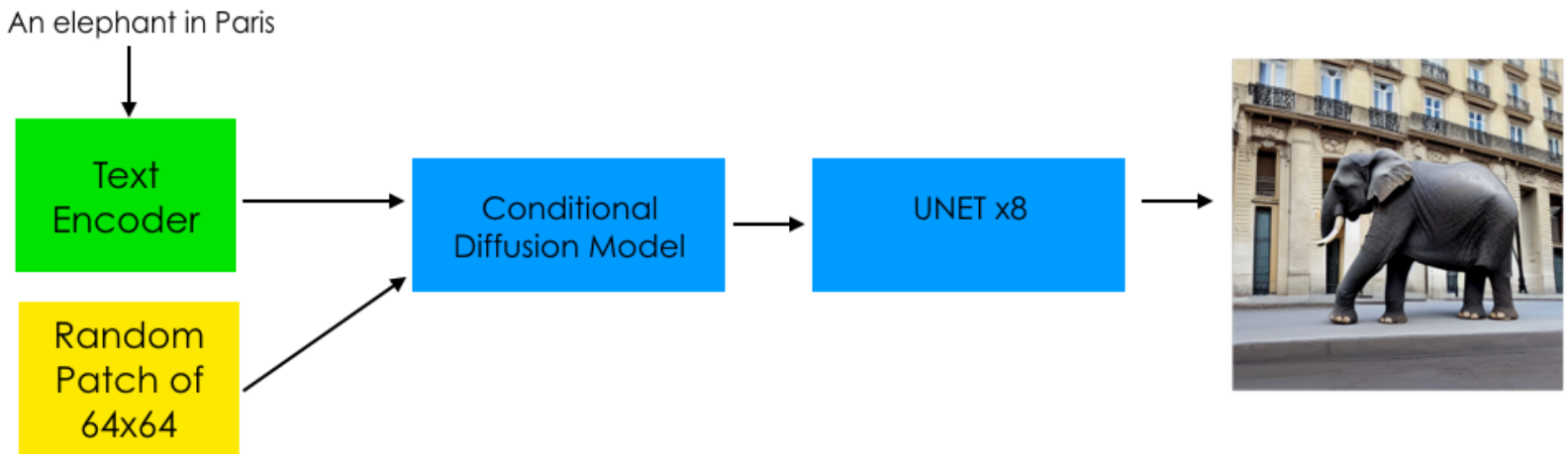


Figure: StableDiffusion

Stable Diffusion models

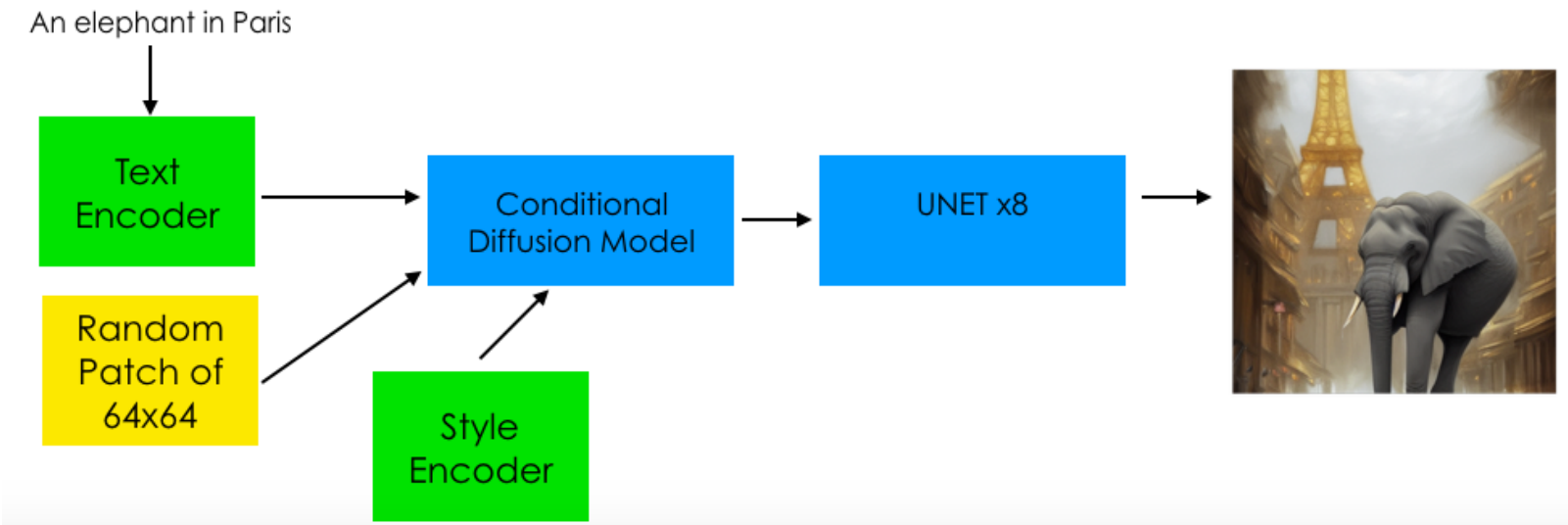


Figure: StableDiffusion

Example: Colab

1. Conditional GANs
   `https://colab.research.google.com/drive/12C-ngdYQrEB8scko6uh9ZQEoQAcpa6uC?usp=sharing`
2. Understanding Diffusion
   `https://colab.research.google.com/drive/1dgml5rx6QKq7LSzwho6oWm7TvEdxgICf?usp=sharing`
3. Stable Diffusion Model
   `https://colab.research.google.com/drive/1xmskXN15B3vK_HtwKy_HNFlKgCPgemiT?usp=sharing`

Contents

1. Introduction
2. Generative models
3. Generative Adversarial Networks (GANs)
4. Variational Diffusion Models
5. References

References I

[Antipov et al., 2017] Antipov, G., Baccouche, M., and Dugelay, J.-L. (2017). Face aging with conditional generative adversarial networks. In *IEEE International Conference on Image Processing (ICIP)*, pages 2089–2093. IEEE.

[Karras et al., 2017] Karras, T., Aila, T., Laine, S., and Lehtinen, J. (2017). Progressive growing of gans for improved quality, stability, and variation. *arXiv preprint arXiv:1710.10196*.

[Shrivastava et al., 2017] Shrivastava, A., Pfister, T., Tuzel, O., Susskind, J., Wang, W., and Webb, R. (2017). Learning from simulated and unsupervised images through adversarial training. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*.